

## 90494 SEARCH REQUEST FORM

Access DB#

Scientific and Technical Information Center

Requester's Full Name: BEN SACKEY Examiner #: 73489 Date: 41/03													
Requester's Full Name: BEN SHENEY Examinet Williams 10./070,36/ Art Unit: 1696 Phone Number 305 - 6889 Serial Number: 10./070,36/ Art Unit: 1696 Phone Number 305 - 6889 Serial Number: 10./070,36/													
Art Unit: 1626 Phone Number 302 6889 Serial Number: 1036 PAPER DISK E-MAIL  Mail Box and Bldg/Room Location: (m. 1. 3 E. 11. Results Format Preferred (circle) PAPER DISK E-MAIL													
If more than one search is submitted, please prioritize searches in order of need:													
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Please provide a detailed statement of the search topic; and describe as specifically as possible to the concept or the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as specifically as possible to the search topic; and describe as possible to the search topic; and the search t													
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Title of Invention: Compositions and therapentic methods invalving 180 flavories													
And or invention. The dian theater et al.													
Inventors (please provide full names): Andrew + peaton et al.													
Earliest Priority Filing Date: 09 10 61 2000													
For Several Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) atong the medical patent authors and the second patent numbers atong the second patent numbers at the second													
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

14 APR 2003 HIGHEST RN 502958-40-9 STRUCTURE FILE UPDATES: DICTIONARY FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002 -

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS L9

139256-07-8 REGISTRY

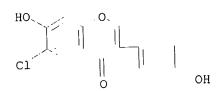
4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) RN CN INDEX NAME)

3D CONCORD FS

C15 H9 C1 O4 MF

SR

BEILSTEIN\*, CA, CAPLUS, CASREACT, TOXCENTER STN Files: (\*File contains numerically searchable property data) LC



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

5 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

1: 137:242178 REFERENCE

2: 137:88466 REFERENCE

134:207652 3: REFERENCE

122:187165 4: REFERENCE

5: 116:105915 REFERENCE

Jan Deleval Reference Librarian Biotechnology & Chemical Library CM1 1507 - 703-308-4498 in et aval@uspio.gov

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(FILE 'REGISTRY' ENTERED AT 11:20:26 ON 15 APR 2003)

1 S L7 NOT L8 L9

FILE 'HCAOLD' ENTERED AT 11:22:22 ON 15 APR 2003

0 S L9 L10

FILE 'USPATFULL, USPAT2' ENTERED AT 11:22:25 ON 15 APR 2003

L11

FILE 'HCAPLUS' ENTERED AT 11:22:31 ON 15 APR 2003

3 S L12 AND (HEATON ? OR KUMAR ? OR KELLY ? OR HUSBAND ?)/AU L12L13

3 S L12 AND NOVOGEN?/PA,CS L14

5 S L12-L14 L15

FILE 'REGISTRY' ENTERED AT 11:23:46 ON 15 APR 2003

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:23:56 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Apr 2003 VOL 138 ISS 16 FILE LAST UPDATED: 14 Apr 2003 (20030414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L15 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS

2002:736111 HCAPLUS ΑN

DN

Isoflavone compounds for inhibition of endothelial cell adhesion molecules and treatment of restenosis and other cardiovascular conditions TI

IN

Husband, Alan; Kelly, Graham Edmund Novogen Research Pty. Ltd., Australia PΑ

PCT Int. Appl., 100 pp. SO

CODEN: PIXXD2

Patent DT

English LA

ICM A61K031-352 ICS A61P009-10 IC

1-8 (Pharmacology)

Section cross-reference(s): 63

FAN.CNT 1

APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_

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20020315
                                               WO 2002-AU288
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
PI WO 2002074307
              GEI, NR, NO, ID, III, IN, IS, OF, AE, NG, AF, AK, NZ, LC, LK, LK, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                               20010316
PRAI AU 2001-3770
                         Α
                               20010626
      AU 2001-5926
      A method is provided for inhibiting expression or activity of an adhesion
OS
      mol. assocd. with an endothelial cell by contacting the adhesion mol. or
AΒ
      endothelial cell with one or more isoflavone compds. or derivs. thereof.
      Also provided are a method of preventing or reducing the risk of
      restenosis after angioplasty, and a method for the treatment or
      prophylaxis of atherosclerosis, coronary artery diseases, other
      cardiovascular diseases, and inflammatory diseases mediated by adhesion
      mols. The invention further provides pharmaceutical compns. useful in
      these methods, as well as methods for the manuf. of such medicaments.
      isoflavone endothelial cell adhesion mol inhibition; restenosis
      angioplasty cardiovascular disease inflammation isoflavone;
      atherosclerosis coronary artery disease isoflavone
       RL: BSU (Biological study, unclassified); BIOL (Biological study)
 ΙT
          (E-; isoflavone compds. for inhibition of endothelial cell adhesion
          mols. and treatment of restenosis and other cardiovascular conditions)
       RL: BSU (Biological study, unclassified); BIOL (Biological study)
  IT
           (LDL; isoflavone compds. for inhibition of endothelial cell adhesion
          mols. and treatment of restenosis and other cardiovascular conditions)
       RL: BSU (Biological study, unclassified); BIOL (Biological study)
  TΤ
           (VCAM-1; isoflavone compds. for inhibition of endothelial cell adhesion
          mols. and treatment of restenosis and other cardiovascular conditions)
           (angina pectoris; isoflavone compds. for inhibition of endothelial cell
       Heart, disease
  ΙT
           adhesion mols. and treatment of restenosis and other cardiovascular
           conditions)
           (angioplasty, restenosis after; isoflavone compds. for inhibition of
  IT
           endothelial cell adhesion mols. and treatment of restenosis and other
           cardiovascular conditions)
           (antiatherosclerotics; isoflavone compds. for inhibition of endothelial
        Antiarteriosclerotics
   IT
           cell adhesion mols. and treatment of restenosis and other
            cardiovascular conditions)
            (atherectomy, direction coronary atherectomy; isoflavone compds. for
        Artery
   IT
            inhibition of endothelial cell adhesion mols. and treatment of
            restenosis and other cardiovascular conditions)
            (coronary; isoflavone compds. for inhibition of endothelial cell
         Artery, disease
   ΙT
            adhesion mols. and treatment of restenosis and other cardiovascular
            conditions)
            (endothelium; isoflavone compds. for inhibition of endothelial cell
         Blood vessel
  . IT
            adhesion mols. and treatment of restenosis and other cardiovascular
```

conditions) Lipoproteins

IT

sackey - 10 / 070361 RL: BSU (Biological study, unclassified); BIOL (Biological study) (high-d.; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions) Anti-inflammatory agents Antihypertensives Antioxidants Atherosclerosis Blood vessel, disease Cardiovascular agents Cell migration Cytotoxic agents Drug delivery systems Human

Hypertension

Inflammation

Transplant and Transplantation

Vasodilators

(isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

Cell adhesion molecules IT

RL: BSU (Biological study, unclassified); BIOL (Biological study) (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

IT Flavones

IT

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses) (isoflavones; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

IT Lipoproteins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (low-d., oxidized; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

IT Lipoproteins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (low-d.; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

ΙT Blood vessel (procedural vascular trauma; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

Artery, disease ΙT (restenosis; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular

conditions) ΙT Blood vessel, disease (small vessel disease; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

ΙT Blood vessel (smooth muscle; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

ΙT Medical goods (stents; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

IT (surgery; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

IT Surgery

(vascular; isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

23531-69-3, .alpha.-Tocopheroxyl radical 1406-18-4, Vitamin E RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

21255-69-6 17238-05-0 486-66-8 491-80-5 485-72-3 446-72-0 81267-65-4 81267-63-2 IT 62845-21-0 40957-83-3, Glycitein 21554-71-2 153409-51-9 145917-93-7 94105-90-5 139256-07-8 88040-00-0 288267-04-9 288267-03-8 288267-00-5 168207-16-7 168207-15-6 351216-89-2, 328406-49-1 328406-47-9 328406-44-6 288267**-**05-0 442150-46-1 Promensil 442150-42-7 442150-43-8 442150-44-9 442150-61-0 442150-54-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD RE.CNT

(1) G J Consultants Pty Ltd; WO 0066576 A 2000 HCAPLUS RE

(2) Johnson & Johnson Consumer Companies Inc; WO 0054753 A 2000 HCAPLUS

(3) Kelly, S; American Journal of Physiology 1998, V274(2 Pt 2), PH513 MEDLINE

(4) May, M; Journal of Pharmacology 1996, V118(7), P1761 HCAPLUS

(5) Novogen Research Pty Ltd; WO 0064438 A 2000 HCAPLUS

(6) Palmetshofer, A; Transplantation 1998, V65(7), P971 HCAPLUS

(7) Protein Technologies InternationalInc; AU 2771400 A1 2000

(8) Schnyder; WO 0016759 A 2000 HCAPLUS

(9) Weber, C; Immunologic research 1996, V15(1), P30 HCAPLUS

TΤ

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL 139256-07-8

(Biological study); USES (Uses) (isoflavone compds. for inhibition of endothelial cell adhesion mols. and treatment of restenosis and other cardiovascular conditions)

4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) 139256-07-8 HCAPLUS RN CN INDEX NAME)

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS

2002:539523 HCAPLUS ΑN

DN

Isoflavones in combination with lipid-regulating agents for regulation of lipids and/or bone density, and compositions therefor ΤI

Husband, Alan James IN

Novogen Research Pty Ltd., Australia

PAPCT Int. Appl., 45 pp. SO CODEN: PIXXD2

Patent DT

English LA

IC

ICS A61K031-352; A61K035-78; A61K031-465; A61P009-10; A61P019-10

1-10 (Pharmacology) CC Section cross-reference(s): 63

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FAN.CNT 1
                                          APPLICATION NO. DATE
                     KIND DATE
    PATENT NO.
                                           _____
                     ____
                                                            20020116
                                          WO 2002-AU42
                            20020718
    WO 2002055072
                      A1
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        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            20010116
PRAI AU 2001-2554
     MARPAT 137:88466
     A method and compns. are provided for regulating bone d. and/or
     circulating lipid levels in a subject which are based on the combined
     administration of at least one isoflavone, or functional deriv., equiv.,
     or analog thereof, and at least one lipid-regulating drug. The method and
     compns. are applicable to the beneficial alteration of blood lipoprotein
     levels, the improvement of vascular compliance, the decrease in the
     propensity of thrombogenic events, the redn. in the risk of vascular
     disease, coronary heart disease, and arteriosclerosis, and to the
     treatment or prevention of osteoporosis.
     cardiovascular drug isoflavone lipid regulating agent combination;
ST
     osteoporosis drug isoflavone lipid regulating agent combination; bone
     density drug isoflavone lipid regulating agent combination; lipid
     regulation agent isoflavone combination
     Sequestering agents
ΙT
        (bile acid-binding; isoflavone combination with lipid-regulating agent
        for regulation of lipids and/or bone d.)
     Artery, disease
ΙT
        (coronary; isoflavone combination with lipid-regulating agent for
        regulation of lipids and/or bone d.)
IT
        (d.; isoflavone combination with lipid-regulating agent for regulation
        of lipids and/or bone d.)
IT
     Lipoproteins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (high-d., cholesterol; isoflavone combination with lipid-regulating
        agent for regulation of lipids and/or bone d.)
     Lipids, biological studies
IT
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
         (hyperlipidemia; isoflavone combination with lipid-regulating agent for
         regulation of lipids and/or bone d.)
      Heart, disease
IT
         (ischemia; isoflavone combination with lipid-regulating agent for
         regulation of lipids and/or bone d.)
      Anti-ischemic agents
 TΤ
      Antiarteriosclerotics
      Anticholesteremic agents
      Anticoagulants
      Arteriosclerosis
      Blood vessel, disease
      Cardiovascular agents
      Drug delivery systems
      Hypercholesterolemia
      Hypolipemic agents
      Osteoporosis
      Thrombosis
         (isoflavone combination with lipid-regulating agent for regulation of
         lipids and/or bone d.)
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- sackey 10 / 070361 Lipids, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) ΙT (isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Flavones RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL IT (Biological study); USES (Uses) (isoflavones; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Lipoproteins RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (low-d., cholesterol; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (resins binding; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) Drug interactions (synergistic; isoflavone combination with lipid-regulating agent for IT regulation of lipids and/or bone d.) (therapeutic agents; isoflavone combination with lipid-regulating agent Osteoporosis IT for regulation of lipids and/or bone d.) Glycerides, biological studies ITRL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (.omega.-3; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 9028-35-7, HMG-CoA reductase RL: BSU (Biological study, unclassified); BIOL (Biological study) IT (inhibitors; isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 57-88-5, Cholesterol, biological studies RL: BSU (Biological study, unclassified); BIOL (Biological study) ΙT (isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.) 59-67-6D, Nicotinic acid, 59-67-6, Nicotinic acid, biological studies IT485-72-3 446-72-0D, analogs and derivs. 446-72-0 486-66-8D, analogs and derivs. 486-66-8 485-72-3D, analogs and derivs. 897-46-1D, analogs 897-46-1 491-80-5D, analogs and derivs. 491-80-5 17238-05-0D, 17238-05-0 943-45-3D, Fibric acid, derivs. and derivs. 17817-31-1D, analogs and derivs. 17817-31-1 analogs and derivs. 21554-71-2D, 21554-71-2 21255-69-6D, analogs and derivs. 21255-69-6 62845-21-0D, analogs and derivs. 62845-21-0 analogs and derivs. 76397-85-8D, analogs and derivs. 76397-85-8 75330-75-5, Lovastatin 79902-63-9, Simvastatin 76397-87-0D, analogs and derivs. 76397-87-0 81267-63-2D, analogs and derivs. 81267-63-2 81093-37-0, Pravastatin 88040-00-0D, 81267-65-4D, analogs and derivs. 88040-00-0 81267-65-4 94105-87-0D, 94105-87-0 93957-54-1, Fluvastatin analogs and derivs. 94105-89-2D, analogs and derivs. 94105-89-2 analogs and derivs. 134523-00-5, Atorvastatin 94105-90-5D, analogs and derivs. 94105-90-5
  - 139256-07-8 139256-07-8D, analogs and derivs. 145917-92-6D, analogs and 145917-92-6 145599-86-6, ·Cerivastatin 145917-93-7D, analogs and derivs. 153409-51-9 145917-93-7 derivs. 168207-15-6D, analogs 168207-15-6 153409-51-9D, analogs and derivs. 168207-16-7D, analogs and derivs. 168207-16-7 and derivs. 288267-03-8 288267-00-5D, analogs and derivs. 288267-00-5 288267-04-9D, analogs 288267-04-9 288267-03-8D, analogs and derivs. 288267-05-0D, analogs and derivs. 288267-05-0 and derivs. 328406-44-6D, analogs and derivs. 328406-47-9 328406-44-6 328406-49-1D, analogs 328406-49-1 328406-47-9D, analogs and derivs. 442150-42-7D, analogs 442150-42-7 351217-32-8, Trinovin and derivs. 442150-43-8D, analogs and derivs. 442150-43-8 and derivs.

442150-44-9 442150-44-9D, analogs and derivs. 442150-46-1

442150-46-1D, analogs and derivs. 442150-54-1 442150-54-1D, analogs

and derivs. 442150-61-0 442150-61-0D, analogs and derivs.

442150-68-7 442150-68-7D, analogs and derivs. 442150-70-1

442150-70-1D, analogs and derivs.

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Bristol-Myers Squibb Company; AU 1022795 A 1995

(2) Bristol-Myers Squibb Company; EP 671170 A 1995 HCAPLUS

(3) Kelly, G; WO 9323069 A 1993 HCAPLUS

(4) Novogen Research Pty Ltd; WO 0064438 A 2000 HCAPLUS

(5) Pfizer Inc; WO 9911260 A 1999 HCAPLUS

(6) Pfizer Products Inc; WO 9911263 A 1999 HCAPLUS

(7) Potter, S; US 5855892 A 1999 HCAPLUS

IT 139256-07-8 139256-07-8D, analogs and derivs.

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(isoflavone combination with lipid-regulating agent for regulation of lipids and/or bone d.)

RN 139256-07-8 HCAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 139256-07-8 HCAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

- L15 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS
- AN 2001:185742 HCAPLUS
- DN 134:207652
- TI Preparation of isoflavones as therapeutic agents with estrogen receptor binding activity
- IN Heaton, Andrew; Kumar, Naresh; Kelly, Graham Edmund; Husband, Alan
- PA Novogen Research Pty. Ltd., Australia
- SO PCT Int. Appl., 44 pp. CODEN: PIXXD2
- DT Patent
- LA English
- IC ICM C07D311-36

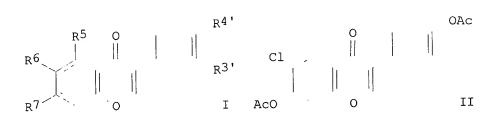
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C07D311-38; C07D471-06; C07C049-215; C07C049-213; A61K031-12;
         A61K031-437; A61P005-00; A61P025-22; A61P025-24; A61P009-10;
         A61P019-10; A61P019-02; A61P017-06; A61P007-00; A61P035-00;
         A61P025-28; A61P017-04; A61P001-00
    26-4 (Biomolecules and Their Synthetic Analogs)
    Section cross-reference(s): 1, 2, 63
FAN.CNT 1
                                                           DATE
                                          APPLICATION NO.
                     KIND
                           DATE
    PATENT NO.
                                          _____
                                                           20000906
                                          WO 2000-AU1056
                           20010315
                      A1
    WO 2001017986
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PΙ W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, SD, SE, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TMYU, ZA, RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG 20000906 BR 2000-13777 BR 2000013777 20020507 Α EP 2000-960231 20000906 20020605 Α1 EP 1210341 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL JP 2001-522209 20000906 T2 20030304 JP 2003508526 NO 2002-1122 20020306 20020326 А NO 2002001122 PRAI AU 1999-2661 19990906 Α

20000906 WO 2000-AU1056 W

OS MARPAT 134:207652

GI



Isoflavanoids, such as I [R3', R4', R7 = H, OH, OAc, etc.; R5 = H, OH, AB OAc, Me, etc.; R6 = H, C1, etc.], were prepd. for pharmaceutical use in the treatment of diseases assocd. with estrogenic or androgenic effects. Thus, isoflavone II was prepd. in 75% yield by acetylation of 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one with acetic anhydride in pyridine. The prepd. isoflavanoids were tested for binding affinity for both subtypes of the estrogen receptor.

isoflavanoid prepn estrogen receptor binding ST

Isoflavonoids IΤ RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for

pharmaceutical use)

IT Estrogen receptors RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process) (prepn. of isoflavones with estrogen receptor binding activity for

pharmaceutical use) 328406-47-9P 328406-45-7P 328406-50-4P 328406-43-5P 328406-42-4P IT 328406-51-5P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for

pharmaceutical use) 81267-53-0 **139256-07-8** RL: BAC (Biological activity or effector, except adverse); BSU (Biological IT study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for

328406-44-6P pharmaceutical use) 81267-67-6P 81267-61-0P 65998-44**-**9P 65998-43-8P 328406-49-1P IT RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of isoflavones with estrogen receptor binding activity for

pharmaceutical use) 328406-52-6

108-73-6, 1,3,5-Benzenetriol RL: RCT (Reactant); RACT (Reactant or reagent) ΙT (prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use)

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD 14 RE.CNT

(1) Anticancer Inc; WO 9848790 Al 1998 HCAPLUS

(2) Bannerjee; J Electrochem Soc India 1998, V47(4), P237 HCAPLUS

(3) Children'S Hospital Oakland Research Institute; WO 9918953 Al 1999 HCAPLUS

(4) Laboratoire L Lafon; WO 0003707 A1 2000 HCAPLUS

(5) Lamberton; Aust J Chem 1978, V31(2), P455 HCAPLUS

(6) Liepa; Aust J Chem 1981, V34(12), P2647 HCAPLUS

(7) Lyonnaise Industrielle Pharmaceutique; FR 2693724 Al 1994 HCAPLUS

(8) New Standard Gmbh; DE 4432947 A1 1996 HCAPLUS

(9) Novogen Research Pty Ltd; WO 9808503 Al 1998 HCAPLUS

(10) Novogen Research Pty Ltd; WO 9936050 Al 1999 HCAPLUS

(11) Ota Isan Kk; JP 01226824 A 1989 HCAPLUS

(12) Wahala; Heterocycles 1989, V28(1), P183 HCAPLUS

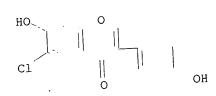
(13) Weidenborner; Phytochemistry 1990, V29(3), P801

(14) Zilliken; US 4157984 1979 HCAPLUS

RL: BAC (Biological activity or effector, except adverse); BSU (Biological TT study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)

(prepn. of isoflavones with estrogen receptor binding activity for pharmaceutical use)

4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) 139256-07-8 HCAPLUS RN CNINDEX NAME)



- L15 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2003 ACS
- 1995:293255 HCAPLUS AN

Synthesis and labeling of isoflavone phytoestrogens, including daidzein 122:187165 DΝ TΙ and genistein

```
Waehaelae, Kristina; Hase, Tapio; Adlercreutz, Herman
     Dep. Chemistry, Univ. Helsinki, Helsinki, FIN-00014, Finland
ΑU
     Proceedings of the Society for Experimental Biology and Medicine (1995),
CS
SO
     208(1), 27-32
     CODEN: PSEBAA; ISSN: 0037-9727
PΒ
     Blackwell
     Journal
DT
     English
LA
     26-4 (Biomolecules and Their Synthetic Analogs)
     The synthesis of the important diphenolic isoflavone type of
CC
     phytoestrogens starting from the corresponding unprotected phenols and
AΒ
     arylacetic acids is discussed. The aryl rings may carry addnl. alkyl,
     methoxy, and/or halogeno groups. Intermediate polyhydroxydeoxybenzoins
     can also be isolated in good yield. Isotopically labeled isoflavone
     phytoestrogens were prepd. by H/D exchange in the complete mol. By this
     method the deuterated products are available in an isotopic purity of
     isoflavone; arylacetate phenol acylation; deuteration daidzein genistein
ST
     Flavonoids
IT
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (iso-, oxo, prepn. and labeling of isoflavones from phenols and
         arylacetic acids)
      104-01-8, 4-Methoxyphenylacetic acid
ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                     136466-47-2P
      104411-13-4P
 IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                                    93-25-4, 2-Methoxyphenylacetic acid
      87-66-1, 1,2,3-Benzenetriol
                                          103-82-2, Phenylacetic acid, reactions
 IT
      95-88-5, 4-Chloro-1,3-benzenediol
                                            108-46-3, 1,3-Benzenediol, reactions
      106-44-5, 4-Methylphenol, reactions
                                                                    120-80-9,
                                     108-95-2, Phenol, reactions
      108-73-6, 1,3,5-Benzenetriol
                                  156-38-7, 4-Hydroxyphenylacetic acid
      1,2-Benzenediol, reactions
      306-08-1, 4-Hydroxy-3-methoxyphenylacetic acid
                                                        504-15-4,
                                 533-73-3, 1,3,4-Benzenetriol 608-25
614-75-5, 2-Hydroxyphenylacetic acid
                                                                 608-25-3,
      5-Methyl-1,3-benzenediol
      2-Methyl-1, 3-benzenediol
                                              1798-09-0, 3-Methoxyphenylacetic
      621-37-4, 3-Hydroxyphenylacetic acid
      acid
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (prepn. of isoflavones from phenols and arylacetic acids)
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                                2491-32-9P
                                             3669-41-8P
                 2491-31-8P
      487-49-0P
 TΨ
                                                 89019-83-0P
                                                              89019-84-1P
                                   77316-95-1P
                     40456-49-3P
      17720-60-4P
                                                                  150295-88-8P
                                                   139256-04-5P
                                   139256-03-4P
                     139256-02-3P
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       (Reactant or reagent)
          (prepn. of isoflavones from phenols and arylacetic acids)
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       446-72-0P, Genistein
                             491-80-5P, 5,7-Dihydroxy-4'-methoxyisoflavone
 TΤ
       486-66-8P, Daidzein
                                                                      13057-72-2P,
                               4044-00-2P, 5,7-Dihydroxyisoflavone
       574-12-9P, Isoflavone
                                                        62845-21-0P
                                           21913-98-4P
                             19725-36-1P
       7-Hydroxyisoflavone
       63909-40-0P, 7-Hydroxy-2'-methoxyisoflavone
                                                                    89019-85-2P
                                                     75187-63-2P
                                    139256-06-7P 139256-07-8P
                      139256-05-6P
       118024-87-6P
       139256-08-9P
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of isoflavones from phenols and arylacetic acids)
       139256-07-8P
  TΤ
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of isoflavones from phenols and arylacetic acids)
       139256-07-8 HCAPLUS
       4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI)
  RN
  CN
       INDEX NAME)
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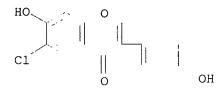
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HO.
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                             ОН
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ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
     1992:105915 HCAPLUS
AN
     116:105915
DN
     Expedient synthesis of polyhydroxyisoflavones
\mathtt{T}\mathtt{T}
     Wahala, Kristiina; Hase, Tapio A.
     Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
ΑU
     Journal of the Chemical Society, Perkin Transactions 1: Organic and
CS
SO
     Bio-Organic Chemistry (1972-1999) (1991), (12), 3005-8
     CODEN: JCPRB4; ISSN: 0300-922X
     Journal
DT
     English
LA
     26-4 (Biomolecules and Their Synthetic Analogs)
CC
     CASREACT 116:105915
     Polyhydroxyisoflavones (19 compds.) were prepd. by reaction of unprotected
OS
     phenols with arylacetic acid in the presence of BF3. Et20 followed by
AΒ
     treatment with MeSO2Cl. In many cases the intermediate deoxybenzoins were
     isoflavone polyhydroxy; deoxybenzoin polyhydroxy; phenol arylacetate
     also isolated.
ST
     condensation
      Flavonoids
TΤ
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (iso-, hydroxy oxo, polyhydroxy-, prepn. of, from unprotected phenols
         and arylacetic acids)
ΙT
      1835-11-6
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (oxidn. of)
                                                           15485-65-1P
                                              3669-41-8P
                  2491-31-8P
                               2491-32-9P
      487-49-0P
                                                  77316-95-1P 89019-83-0P
 IT
                                   52122-86-8P
                     40456-49-3P
      17720-60-4P
                                                                   139256-03-4P
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                                   139256-01-2P
                     92549-46-7P
      89019-84-1P
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      (Reactant or reagent)
          (prepn. and intramol. cyclocondensation of)
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 IT
      (Reactant or reagent)
          (prepn. and reaction of, with phenols)
      67736-18-9P
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      RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of)
                                                         574-12-9P, Isoflavone
                                           491-80-5P
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       446-72-0P
 TT
                                                                32684-57-4P
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                                                  89019-85-2P
                                    75187-63-2P
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                                                   139256-08-9P
                      139256-06-7P 139256-07-8P
       139256-05-6P
       RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of, from phenol and phenylacetic acid)
                                             103-82-2, Phenylacetic acid,
       93-25-4, 2-Methoxyphenylacetic acid
                   104-01-8, 4-Methoxyphenylacetic acid 156-38-7,
  IT
       4-Hydroxyphenylacetic acid 614-75-5, 2-Hydroxyphenylacetic acid 621-37-4, 3-Hydroxyphenylacetic acid 1798-09-0, 3-Methoxyphenylacetic
       621-37-4, 3-Hydroxyphenylacetic acid
       acid
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          (reaction of, with phenols)
                                      95-88-5, 4-Chloro-1,3-benzenediol
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87-66-1, 1,2,3-Benzenetriol

ΙT

106-44-5, p-Cresol, reactions 108-46-3, m-Hydroquinone, reactions 108-73-6, 1,3,5-Benzenetriol 108-95-2, Phenol, reactions 120-80-9, o-Hydroquinone, reactions 123-31-9, p-Hydroquinone, reactions 504-15-4, 5-Methyl-1,3-benzenediol 533-73-3, 1,3,4-Benzenetriol 608-25-3, 2-Methyl-1,3-benzenediol RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with phenylacetic acids) 139256-07-8P
RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, from phenol and phenylacetic acid) 139256-07-8 HCAPLUS 4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA



INDEX NAME)

ΙT

RN

CN

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STRUCTURE FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9 DICTIONARY FILE UPDATES: 14 APR 2003 HIGHEST RN 502958-40-9

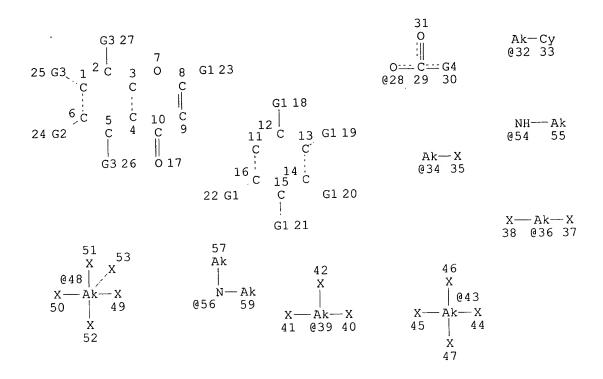
TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting  ${\tt SmartSELECT}$  searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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VAR G1=H/OH VAR G2=H/X VAR G3=H/OH/AK/28 VAR G4=H/AK/34/36/39/43/48/NH2/54/56/32 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 58

STEREO ATTRIBUTES: NONE L18 169 SEA FILE=REGISTRY SUB=L2 CSS FUL L16

100.0% PROCESSED 6958 ITERATIONS 169 ANSWERS SEARCH TIME: 00.00.01

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L11
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L12
              5 S L9
L13
              3 S L12 AND (HEATON ? OR KUMAR ? OR KELLY ? OR HUSBAND ?)/AU
              3 S L12 AND NOVOGEN?/PA,CS
L14
L15
              5 S L12-L14
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             11 S L19 AND C15H1006
L20
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L21
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L23
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L24
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     FILE 'HCAPLUS' ENTERED AT 11:40:12 ON 15 APR 2003
L26
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L27
L28
             12 S L26 AND NOVOGEN?/PA,CS
L29
             21 S L27, L28
           2704 S L26 AND (PD<=19990906 OR PRD<=19990906 OR AD<=19990906)
L30
             14 S L29 AND L30
L31
                E W02000-AU1056/AP, PRN
              1 S E3, E4
L32
L33
              1 S L32 AND L26
                E ESTROGEN RECEPTOR/CT
L34
           8369 S E11-E18
                E E11+ALL
          13813 S E12, E11+NT
L35
L36
             86 S L30 AND L34, L35
L37
             14 S L31, L33
              1 S L37 AND L34, L35
L38
L39
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            191 S L42
L43
L44
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L46
              2 S L44 AND ?ESTROGEN? (L) RECEPTOR
L47
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45 S L44 AND P/DT
L48
             18 S L48 AND US/PC
L49
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L50
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=> d ide can 121

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L21 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
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     4H-1-Benzopyran-4-one, 3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-
RN
CN
     (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
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Isoflavone, 3',4',5,7-tetrahydroxy- (7CI, 8CI)

OTHER NAMES:

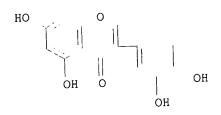
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Orobol CN

3D CONCORD FS

MF

N Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CHEMCATS, DDFU, DRUGU, EMBASE, C15 H10 O6 STN Files: LCMEDLINE, NAPRALERT, RTECS\*, TOXCENTER, USPATFULL (\*File contains numerically searchable property data)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

94 REFERENCES IN FILE CA (1962 TO DATE) 94 REFERENCES IN FILE CAPLUS (1962 TO DATE) 3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

LZI and LZZ ! are excluded : as per Groniso 1: 138:175571 REFERENCE 138:95264 2: REFERENCE 138:69917 3: REFERENCE 137:329286 REFERENCE 4: 137:252731 REFERENCE 5:

137:226166 6: REFERENCE

137:37406 7: REFERENCE

136:374545 8: REFERENCE

136:345763 9: REFERENCE

136:196995 REFERENCE 10:

=> d ide can 123

L23 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 155955-25-2 REGISTRY

CN 4H-1-Benzopyran-4-one, 5-hydroxy-7-methyl-3-phenyl- (9CI) (CA

INDEX NAME)

FS 3D CONCORD MF C16 H12 O3

SR CA

LC STN Files: CA, CAPLUS

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1962 TO DATE)

1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 121:280544

=> s 140 not 142

L51 3 L40 NOT L42

=> d ide can tot

L51 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS

RN 574-12-9 REGISTRY

CN 4H-1-Benzopyran-4-one, 3-phenyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Isoflavone (6CI, 7CI, 8CI)

OTHER NAMES:

CN 3-Phenylchromone

FS 3D CONCORD

MF - C15 H10 O2

CI COM

LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CIN, CSCHEM, DDFU, DRUGU, EMBASE, HODOC\*, IFICDB, IFIPAT, IFIUDB, MRCK\*, NAPRALERT, PIRA, PROMT, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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                12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)
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 REFERENCE
              2: 138:203825
 REFERENCE
             3: 138:152800
 REFERENCE
             4: 138:152532
                                                       Jeteluded
these 3 cmpds
from Biblios.
search
 REFERENCE
             5: 138:152521
 REFERENCE
             6: 138:126767
 REFERENCE
             7: 138:122018
 REFERENCE
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 REFERENCE
             9: 138:89093
 REFERENCE 10: 138:72288
L51 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS
     486-66-8 REGISTRY
     4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
CN
     NAME)
OTHER CA INDEX NAMES:
    Daidzein (6CI)
     Isoflavone, 4',7-dihydroxy- (8CI)
OTHER NAMES:
CN
    4',7-Dihydroxyisoflavone
     7,4'-Dihydroxyisoflavone
CN
    7-Hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one
CN
CN
     Daidzeol
CN
     K 251b
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     NPI 031E
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MF
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CI
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                 ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*,
      BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,
      CASREACT, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DDFU,
      DRUGU, DRUGUPDATES, EMBASE, HODOC*, IFICDB, IFIPAT, IFIUDB, IPA,
      MEDLINE, MRCK*, NIOSHTIC, PROMT, RTECS*, SPECINFO, TOXCENTER, USPAT2,
        (*File contains numerically searchable property data)
    Other Sources: EINECS**
        (**Enter CHEMLIST File for up-to-date regulatory information)
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## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1655 REFERENCES IN FILE CA (1962 TO DATE) 30 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA 1666 REFERENCES IN FILE CAPLUS (1962 TO DATE) 24 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

138:247754 1: REFERENCE

138:237329 REFERENCE 2:

3: 138:231731 REFERENCE

138:220683 4: REFERENCE

138:220511 5: REFERENCE

138:217754 REFERENCE 6:

138:217309 7: REFERENCE

138:214863 8: REFERENCE

138:204084 9: REFERENCE

REFERENCE 10: 138:198885

L51 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2003 ACS

4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

OTHER CA INDEX NAMES:

Genistein (6CI)

Isoflavone, 4',5,7-trihydroxy- (8CI) CN

OTHER NAMES:

4',5,7-Trihydroxyisoflavone CN

5,7,4'-Trihydroxyisoflavone CN

Baichanin A CN

C.I. 75610 CN

Genisteol CN

Genisterin CN

NPI 031L CN

Prunetol CN

SIPI 807-1 CN

Sophoricol CN

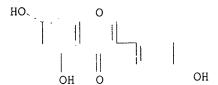
3D CONCORD FS

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ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN\*, COM BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM, CSNB, DDFU, DRUGU, STN Files: LC EMBASE, HODOC\*, IPA, MEDLINE, MRCK\*, NAPRALERT, NIOSHTIC, PIRA, PROMT, RTECS\*, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)
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 (\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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34 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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REFERENCE 7: 138:231519

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=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 11:48:31 ON 15 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 15 Apr 2003 VOL 138 ISS 16 FILE LAST UPDATED: 14 Apr 2003 (20030414/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L50 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2003 ACS
      2001:185742 HCAPLUS
      Preparation of isoflavones as therapeutic agents with estrogen
AN
DN
TΙ
      receptor binding activity
      Heaton, Andrew; Kumar, Naresh; Kelly, Graham
      Edmund; Husband, Alan
      Novogen Research Pty. Ltd., Australia
PΑ
      PCT Int. Appl., 44 pp.
SO
       CODEN: PIXXD2
       Patent
 DT
       English
       ICS C07D311-38; C07D471-06; C07C049-215; C07C049-213; A61K031-12;
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             A61P019-10; A61P019-02; A61P017-06; A61P007-00; A61P035-00;
             A61P025-28; A61P017-04; A61P001-00
        26-4 (Biomolecules and Their Synthetic Analogs)
        Section cross-reference(s): 1, 2, 63
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                                                       APPLICATION NO.
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                             KIND DATE
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        PATENT NO.
                                                                            20000906 <--
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                                Α
                                                  <--
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                                W
          WO 2000-AU1056
          MARPAT 134:207652
    OS
    GΙ
                                                                       OAc
                                  R4'
            R5
                                                        1
                                           Cl
```

<sub>R</sub>3'

AcO

II

```
Isoflavanoids, such as I [R3', R4', R7 = H, OH, OAc, etc.; R5 = H, OH,
AB
    OAc, Me, etc.; R6 = H, C1, etc.], were prepd. for pharmaceutical use in
     the treatment of diseases assocd. with estrogenic or androgenic
     effects. Thus, isoflavone II was prepd. in 75% yield by acetylation of
     6-chloro-7-hydroxy-3-(4-hydroxyphenyl)-4H-1-benzopyran-4-one with acetic
     anhydride in pyridine. The prepd. isoflavanoids were tested for binding
     affinity for both subtypes of the estrogen receptor.
     isoflavanoid prepn estrogen receptor binding
ST
     Isoflavonoids
IT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL
     (Biological study); RACT (Reactant or reagent); USES (Uses)
        (prepn. of isoflavones with estrogen receptor
        binding activity for pharmaceutical use)
     Estrogen receptors
TΤ
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (prepn. of isoflavones with estrogen receptor
        binding activity for pharmaceutical use)
                                                  328406-47-9P
                                                                  328406-50-4P
                                   328406-45-7P
                    328406-43-5P
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     study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
     (Reactant or reagent); USES (Uses)
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                                             139256-07-8
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                    65998-44-9P
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ΙT
                                   328406-49-1P
      328406-46-8P · 328406-48-0P
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               THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
 RE.CNT 14
 RE
 (1) Anticancer Inc; WO 9848790 A1 1998 HCAPLUS
 (2) Bannerjee; J Electrochem Soc India 1998, V47(4), P237 HCAPLUS
 (3) Children'S Hospital Oakland Research Institute; WO 9918953 A1 1999 HCAPLUS
 (4) Laboratoire L Lafon; WO 0003707 Al 2000 HCAPLUS
 (5) Lamberton; Aust J Chem 1978, V31(2), P455 HCAPLUS
 (6) Liepa; Aust J Chem 1981, V34(12), P2647 HCAPLUS
 (7) Lyonnaise Industrielle Pharmaceutique; FR 2693724 Al 1994 HCAPLUS
 (8) New Standard Gmbh; DE 4432947 Al 1996 HCAPLUS
 (9) Novogen Research Pty Ltd; WO 9808503 Al 1998 HCAPLUS
 (10) Novogen Research Pty Ltd; WO 9936050 Al 1999 HCAPLUS
 (11) Ota Isan Kk; JP 01226824 A 1989 HCAPLUS
 (12) Wahala; Heterocycles 1989, V28(1), P183 HCAPLUS
 (13) Weidenborner; Phytochemistry 1990, V29(3), P801
 (14) Zilliken; US 4157984 1979 HCAPLUS
      62845-21-0
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study, unclassified); RCT (Reactant); THU (Therapeutic use); BIOL

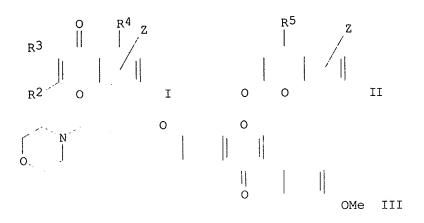
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RN
CN
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      ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2003 ACS
 L50
      2001:185741 HCAPLUS
      Preparation of flavones, xanthones, and coumarins for pharmaceutical use
 AN
 DN
      in the treatment of cancer
 ΤI
       Bombardelli, Ezio; Valenti, Piero
 IN
       Indena S.p.A., Italy
  PA
       PCT Int. Appl., 46 pp.
  SO
       CODEN: PIXXD2
  DT
       Patent
       English
       ICS C07D311-36; C07D311-16; C07D311-86; A61K031-37; A61P035-00
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       ICM C07D311-30
  IC
       26-4 (Biomolecules and Their Synthetic Analogs)
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                          KIND DATE
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                                  20021205
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20000828

W

WO 2000-EP8365 MARPAT 134:207651

OS GI



AB Flavones, xanthones, and coumarins, such as I and II [Z = OCH2C.tplbond.CCH2NRR1; R, Rl = H, alkyl; NRR1 = nitrogen contg. heterocyclyl, such as 1-piperidinyl or 4-morpholinyl; R2, R3 = H, substituted aryl, such as hydroxyphenyl, etc.; R4 = H, OH, alkoxy, etc.; R5 = H, alkyl], were prepd. for pharmaceutical use as modulators of multiple drug resistance in cancer chemotherapy and for possible use in the treatment or prevention of other disorders, such as menopausal disorders and osteoporosis. Thus, isoflavone deriv. III was prepd. by reacting 7-hydroxy-4'-methoxyisoflavone with propargyl bromide using K2CO3 and KI in acetone to form 7-(2-propynyloxy)-4'-methoxyisoflavone, which was then reacted with formaldehyde and morpholine using CuSO4 in EtOH and H2O to form III. The prepd. compds. were tested for cytotoxicity against drug resistant breast cancer cells MDA-435/LCC6-MDR.

ST flavone xanthone coumarin prepn antitumor agent

IT Antitumor agents

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

IT Flavonoids

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

328564-16-5P 328564-17-6P 328564-18-7P 328564-19-8P ΙT 67268-57-9P 328564-24-5P 328564-20-1P 328564-21-2P 328564-22-3P 328564-23-4P 328564-29-0P 328564-27-8P 328564-28-9P 328564-25-6P 328564-26-7P

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

1T 90-33-5 106-96-7 109-89-7, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 485-72-3 486-66-8 491-80-5 719-41-5 1915-98-6 2759-28-6 3722-51-8 6665-86-7 13004-42-7 13057-72-2 18651-15-5

3722-51-8 6665-86-7 13004-42-7 **13057-72-2** 18653 RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in the treatment of cancer)

The treatment of Cancer)

1T 67091-11-6P 67268-43-3P 124039-97-0P 328564-08-5P,

7-(2-Propynyloxy)-4'-methoxyisoflavone 328564-09-6P 328564-10-9P
328564-11-0P 328564-12-1P 328564-13-2P 328564-14-3P 328564-15-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of flavones, xanthones, and coumarins for pharmaceutical use in

```
sackey - 10 / 070361
        the treatment of cancer)
RE.CNT
              THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Allergan Inc; EP 0419132 A 1991 HCAPLUS
(2) Allergan Inc; WO 9518803 A 1995 HCAPLUS
(3) Francois, M; US 4151291 A 1979 HCAPLUS
(4) Jay, P; US 3513198 A 1970
(5) Petrow, V; JOURNAL OF PHARMACY AND PHARMACOLOGY 1958, V10, P86 HCAPLUS
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     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
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ΑN

2000:756511 HCAPLUS

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DN
     133:317571
ΤI
     Estrogen receptor-.beta. ligands for therapy
     Barlaam, Bernard Christophe; Piser, Timothy Martin
PΑ
     Astrazeneca AB, Swed.
SO
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     CODEN: PIXXD2
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     1-12 (Pharmacology)
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ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2003 ACS

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PRAI US 1999-129901P
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                            20000411
     WO 2000-GB1380
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     A method for treating a disease assocd. With the estrogen
OS
     receptor (ER) - . beta. comprises the step of administering a
AB
     therapeutically effective amt. of estrogen receptor
     -.beta.-selective ligands, which mimic estrogen replacement
     therapy (ERT), but lack undesirable side effects of ERT. The ligand
     satisfies the equation: (Ki.alpha.A/Ki.beta.A)/(Ki.alpha.E/Ki.beta.E) > 1,
     where Ki.alpha.A and Ki.beta.A are the Ki values for the agonists in
     ER-.alpha. and ER-.beta., and Ki.alpha.E and Ki.beta.E are the Ki values
     for estrogens in ER-.alpha. and ER-.beta., resp. Diseases
      assocd. with the ER-.beta. are Alzheimer's disease, anxiety, depression,
      osteoporosis, cardiovascular disease, rheumatoid arthritis, and prostate
      cancer. For example, (3-bromo-4-hydroxyphenyl)-5,7-dihydroxy-5H-1-
      benzopyran-4-one was prepd. using 1,3,5-trihydroxybenzaldehyde and
      3-bromo-4-hydroxyphenylacetic acid as starting compds.
      estrogen receptor ligand Alzheimer disease;
      antidepressant anxiolytic estrogen receptor ligand;
 ST
      antirheumatic estrogen receptor ligand; osteoporosis
      cardiovascular disease estrogen receptor ligand;
      prostate cancer estrogen receptor ligand
      Anti-Alzheimer's agents
 IT
      Antidepressants
      Antirheumatic agents
       Anxiolytics
          (estrogen receptor-.beta. ligands for treatment of
       Cardiovascular agents
          cardiovascular and neurol. disorders, rheumatoid arthritis,
          osteoporosis and prostate cancer)
       Estrogens
  ΤT
       RL: BAC (Biological activity or effector, except adverse); BSU (Biological
       study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
       BIOL (Biological study); PREP (Preparation); USES (Uses)
           (estrogen receptor-.beta. ligands for treatment of
          cardiovascular and neurol. disorders, rheumatoid arthritis,
           osteoporosis and prostate cancer)
        Hormone replacement therapy
           (mimicking; estrogen receptor-.beta. ligands for
  IT
           treatment of cardiovascular and neurol. disorders, rheumatoid
           arthritis, osteoporosis and prostate cancer)
        Prostate gland
   IT
           (neoplasm, inhibitors; estrogen receptor-.beta.
        Prostate gland
           ligands for treatment of cardiovascular and neurol. disorders,
           rheumatoid arthritis, osteoporosis and prostate cancer)
            (prostate gland; estrogen receptor-.beta. ligands
        Antitumor agents
   IT
            for treatment of cardiovascular and neurol. disorders, rheumatoid
            arthritis, osteoporosis and prostate cancer)
         Osteoporosis
            (therapeutic agents; estrogen receptor-.beta.
    IT
```

ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL IT (Biological study); PROC (Process) (.beta.; estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 6468-98-0P 5217-90-3P 6468-36-6P 5217-89-0P 480-23-9P 552-59**-**0P IT 18651-39-3P 18651-11-1P 15584-09-5P 15584-08-4P 13111-57-4P 36190-95-1P 31913-52-7P 24051-97-6P 24051-96-5P 21554-71-2P 63046-09-3P 62845-09-4P 62845-21-0P 40624-03-1P 94105-90-5P 91805-21-9P 67295-48-1P **70943-68-9P** 101068-34-2P 101068-31-9P 96462-61-2P **96657-99-7P** 303012-54-6P 299951-78-3P 215435-34-0P 157405-88-4P 123731-49-7P 303012-59-1P 303012-58-0P 303012-57-9P 303012-56-8P 303012-55-7P 303012-64-8P 303012-63-7P 303012-62-6P 303012-61-5P 303012-60-4P 303012-67-1P 303012-66-0P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (estrogen receptor -. beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 156-38-7, 4-Hydroxyphenylacetic acid 487-70-7, 38692-80-7, 3-Bromo-4-hydroxyphenylacetic IT 2,4,6-Trihydroxybenzaldehyde acid RL: RCT (Reactant); RACT (Reactant or reagent) (estrogen receptor -. beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 303012-69-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT IT (Reactant or reagent) (estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 62845-21-0P 70943-68-9P 96657-99-7P RL: BAC (Biological activity or effector, except adverse); BSU (Biological ΙT study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (estrogen receptor-.beta. ligands for treatment of cardiovascular and neurol. disorders, rheumatoid arthritis, osteoporosis and prostate cancer) 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-5-methyl- (9CI) (CA RN CN INDEX NAME)

RN 70943-68-9 HCAPLUS CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

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HO.
                  OH
RN
     96657-99-7 HCAPLUS
CN
     4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX
     NAME)
HO.
           0
                       OH
      OH
    ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1999:597471 HCAPLUS
ΑN
     131:199621
DN
TI
    Multi-step preparation of high-purity ipriflavone
ΙN
     Ferrari, Massimo
PA
     Erregierre S.p.A., Italy
SO
     Eur. Pat. Appl., 10 pp.
     CODEN: EPXXDW
DT
     Patent
LA
     English
IC
     ICM C07D311-36
     ICS A61K031-35
     27-14 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 26, 63
FAN.CNT 1
                                           APPLICATION NO.
     PATENT NO.
                      KIND DATE
                                                            DATE
     EP 941992
PΙ
                      A1
                            19990915
                                           EP 1999-103494
                                                            19990223 <--
     EP 941992
                      В1
                            20020508
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
     IT 1298619
                      В1
                            20000112
                                           IT 1998-MI483
                                                            19980310 <--
     US 5973169
                       Α
                            19991026
                                           US 1999-255043
                                                             19990222 <--
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                                           JP 1999-60451
                                                             19990308 <--
PRAI IT 1998-MI483
                            19980310
                       Α
                                     <--
    CASREACT 131:199621
OS
AΒ
     Ipriflavone, a calcium regulator used in the treatment of osteoporosis (no
     data), is prepd. in high yield and selectivity by: (A) the
     cyclocondensation of 2,4-dihydroxyphenyl benzyl ketone (I) with Et
     orthoformate in DMF at 115-120.degree. using a I wt./solvent vol. (w/v)
     ratio of <1/4 and in the presence of morpholine as a catalyst to yield
     7-hydroxyisoflavone (II); (B) sepn. of II from the reaction residue by its
     pptn. as its corresponding dicyclohexylamine salt, followed by
     neutralization with orthophosphoric acid to yield II; and (C)
     etherification of II with an iso-Pr halide (e.g., iso-Pr bromide) to give
     ipriflavone contg. .ltoreq.0.1% impurity.
ST
    ipriflavone manuf high purity; cyclocondensation manuf high purity
     ipriflavone; etherification manuf high purity ipriflavone
ΙT
     Precipitation (chemical)
        (of 7-hydroxyisoflavone dicyclohexylamine salt in the prepn. of
```

```
high-purity ipriflavone)
ΙT
     Etherification
        (of 7-hydroxyisoflavone with iso-Pr bromide in the manuf. of
        high-purity ipriflavone)
IT
     Cyclocondensation reaction
        (of benzyl 2,4-dihydroxyphenyl ketone with Et orthoformate in the
        prepn. of 7-hydroxyisoflavone)
ΙT
     110-91-8, Morpholine, uses
     RL: CAT (Catalyst use); USES (Uses)
        (multi-step prepn. of high-purity ipriflavone)
IT
     13057-72-2P, 7-Hydroxyisoflavone 241804-59-1P
     RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
IT
     35212-22-7P, Ipriflavone
     RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
     (Preparation)
        (multi-step prepn. of high-purity ipriflavone)
IT
     75-26-3, Isopropyl bromide
                                  101-83-7, Dicyclohexylamine
                                                                 7664-38-2,
    Orthophosphoric acid, reactions
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
IT
     122-51-0, Ethyl orthoformate
                                   3669-41-8, 2,4-Dihydroxyphenyl benzyl
     ketone
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone from)
                     78-83-1, Isobutyl alcohol, uses
TΤ
     68-12-2, uses
                                                      108-88-3, Toluene, uses
     7732-18-5, Water, uses
    RL: NUU (Other use, unclassified); USES (Uses)
        (solvent; multi-step prepn. of high-purity ipriflavone)
RE.CNT
              THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; WO 15 1991 HCAPLUS
(2) Chinoin; WO 9115483 A 1991 HCAPLUS
(3) Szerves Vegyipari Fejleszto Kosos Vallalat; HU 55376 A HCAPLUS
    13057-72-2P, 7-Hydroxyisoflavone 241804-59-1P
    RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
    preparation); PREP (Preparation); RACT (Reactant or reagent)
        (multi-step prepn. of high-purity ipriflavone)
RN
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
          O.
                Ph
RN
    241804-59-1 HCAPLUS
    4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, compd. with
CN
    N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)
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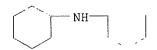
CRN 13057-72-2 CMF C15 H10 O3

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CM

CM 2

CRN 101-83-7 CMF C12 H23 N



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L50 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2003 ACS
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AN 1997:113419 HCAPLUS

126:122303 DN

Hair growth promoting compositions containing isoflavanoid derivatives TI

ΙN Kung, Patrick C.; Li, Ze Zeng

PΑ Kung, Patrick, C., USA

SO PCT Int. Appl., 20 pp.

CODEN: PIXXD2

DTPatent

LA English

ICM A01N043-16 ICS A61K031-35 IC

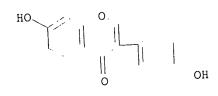
62-3 (Essential Oils and Cosmetics) CC Section cross-reference(s): 1, 26, 63

FAN.	CNT	1																
	PATENT NO.				KIND		DATE			APPLICATION NO. DATE								
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		W:													FI,			
			IS,	JP,	KG,	KP,	KR,	ΚZ,	LK,	LR,	LS,	LT,	LV,	MD,	MG,	MK,	MN,	MX,
															UA,			
			AZ,	BY														
		RW:													FI,			
			IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,
			MR,	NE,	SN,	TD,	TG											
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	AU 9659704			A	1	1996	1230		AU 1996-59704						19960603 <			
PRAI	AI US 1995-484097 US 1996-659466 WO 1996-US8433					19950607			<									
				19960531			<	<										
				19960603			<-	<										
00	MATA	ייי עכוכ	126.	1223	<b>Λ</b> 3													

OS MARPAT 126:122303

Novel compns. of isoflavanoid derivs. useful for the treatment of male AΒ pattern baldness and alopecia areata, promoting the conversion of gray hair to the original pigment in hair follicles, and increasing the blood supply to the brain are disclosed. The invention also relates to methods for treatment of male pattern baldness and alopecia areata, gray hair, and brain circulatory deficiencies. Sodium methoxide 6.48 was added to 50 mL DMF and the mixt. was distd. to eliminate alc. then, resulting product was cooled to .ltoreq.20.degree.. Dimethylamino-methoxy sulfuric acid Me ester (prepn. given) was added dropwise to the cooled product and the

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mixt. was allowed to react for 5 h. The reaction mixt. was distd. to
    remove dimethyllformaide from the mixt. followed by addn. of water to
    obtain daidzein (I). A tablet contained I 100, lactose 50, starch 23,
    microcryst. cellulose 2, dicalcium phosphate 30 mg, surfactants trace, and
    magnesium trace. The efficacy of tablets (2 tablet 3 times/day) in
    treatment of hypertensive male bald subject is reported.
    hair growth promoter isoflavanoid deriv; pharmaceutical tablet daidzein
ST
    male baldness
        (areata; hair growth promoting compns. contg. isoflavanoid derivs.)
    Alopecia
IT
        (cerebrovascular; hair growth promoting compns. contg. isoflavanoid
     Brain, disease
IT
        derivs.)
     RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
IT
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (growth stimulants; hair growth promoting compns. contg. isoflavanoid
     (Uses)
        derivs.)
     Isoflavonoids
     RL: RCT (Reactant); RACT (Reactant or reagent)
IT
         (hair growth promoting compns. contg. isoflavanoid derivs.)
         (male pattern; hair growth promoting compns. contg. isoflavanoid
      Alopecia
 IΤ
         derivs.)
         (ointments, creams; hair growth promoting compns. contg. isoflavanoid
      Drug delivery systems
 ΙT
         derivs.)
         (ointments; hair growth promoting compns. contg. isoflavanoid derivs.)
      Drug delivery systems
 IT
         (tablets; hair growth promoting compns. contg. isoflavanoid derivs.)
      Drug delivery systems
 IT
                 486-63-5P 486-66-8P, Daidzein 19725-36-1P
                                              142574-14-9P
      485-72-3P
                               139256-06-7P
 ΙT
      56401-04-8P 89019-85-2P
                                                186246-61-7P
      146307-82-6P 148356-24-5P 186246-60-6P
                                               186246-65-1P
      186246-62-8P 186246-63-9P 186246-64-0P
                                                    186246-69-5P
       RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
                                     186246-68-4P
       (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
          (hair growth promoting compns. contg. isoflavanoid derivs.)
       (Uses)
                           75-93-4, Methyl sulfate
       68-12-2, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
  TΤ
          (hair growth promoting compns. contg. isoflavanoid derivs.)
       486-66-8P, Daidzein 19725-36-1P 89019-85-2P
       148356-24-5P 186246-60-6P 186246-63-9P
  IT
       RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); THU
        (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
           (hair growth promoting compns. contg. isoflavanoid derivs.)
        (Uses)
        4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
        486-66-8 HCAPLUS
   RN
```



CN

NAME)

19725-36-1 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX CN NAME)

89019-85-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN

148356-24-5 HCAPLUS

4H-1-Benzopyran-4-one, 5-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

186246-60-6 HCAPLUS

4H-1-Benzopyran-4-one, 7-(acetyloxy)-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

186246-63-9 HCAPLUS

4H-1-Benzopyran-4-one, 5-(acetyloxy)-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RNCN NAME)

186246-64-0 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-(acetyloxy)-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN

L50 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1993:575863 HCAPLUS AN

DN

Isoflavones from soybean exudates inducing nodulation of Bradyrhizobium TIjaponicum.

Kosslak, Renee; Bookland, Roger; Appelbaum, Edward R. ΙN

Lubrizol Genetics, Inc., USA PA

U.S., 15 pp. Cont. of U.S. Ser. No. 35,516, abandoned. SO CODEN: USXXAM

Patent DΤ

English LA

ICM A01N063-00 ICS A01N043-00; C12R001-41; C12N001-00; C05F011-08; A01C001-06 IC

424-93A NCL

5-2 (Agrochemical Bioregulators) CC Section cross-reference(s): 3, 10, 11

FAN.CNT 1

APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ \_\_\_\_ \_\_\_\_\_ US 1989-393081 19890809 <--19930720 US 5229113 Α

19870407 <--PRAI US 1987-35516

The isoflavones daidzein and genistein of soybean exudates are identified as inducers of nodulation of Bradyrhizobium. These compds. can be used for regulated induction of nodulation or for expression of heterologous genes under expression of the nodulation promoter. Several other flavonoids are also identified as inducers, with daidzein and genistein effective at .ltoreq.1.mu.M. The compds. were identified by chromatog. fractionation of exudates and assaying fractions for induction of expression of a reporter gene from the nod promoter.

Bradyrhizobium nodulation inducer flavone soybean ST

Bradyrhizobium japonicum IT

(nodulation by, induction of, flavones from soybean exudates for)

IT

Flavonoids RL: BIOL (Biological study) (nodulation inducers, by Bradyrhizobium japonicum, induction of nodABC genes by)

ΙT Soybean

(nodulation inoculum for, Bradyrhizobium japonicum and nodulation-inducing flavones in)

Flavonoids IT

RL: BIOL (Biological study)
(iso-, oxo, nodulation inducers, by Bradyrhizobium japonicum, induction of nodABC genes by)

IT Operon

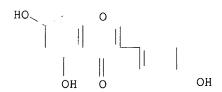
(nodABCIJ, induction of, flavones for)

IT 446-72-0, Genistein 479-13-0, Coumestrol 485-72-3, Formononetin 486-66-8, Daidzein 491-80-5, Biochanin A 520-18-3, Kaempferol 520-36-5, Apigenin 2196-14-7 4044-00-2, 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone RL: BIOL (Biological study) (nodulation inducer, by Bradyrhizobium japonicum, induction of nodABC genes by)

IT 446-72-0, Genistein 486-66-8, Daidzein 4044-00-2
, 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone
RL: BIOL (Biological study)
 (nodulation inducer, by Bradyrhizobium japonicum, induction of nodABC genes by)

RN 446-72-0 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 486-66-8 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

RN 4044-00-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)

RN 13057-72-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

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HO O Ph
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ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2003 ACS
    1993:535006 HCAPLUS
    119:135006
DN
    Carbon dioxide detector
TI
    Mills, Andrew; Chang, Qing
TN
    Johnson and Johnson Professional Products Ltd., UK
PA
     PCT Int. Appl., 19 pp.
SO
    CODEN: PIXXD2
DT
     Patent
     English
LA
     ICM G01N031-22
IC
     9-1 (Biochemical Methods)
CC
FAN.CNT 1
                                           APPLICATION NO. DATE
                      KIND DATE
     PATENT NO.
                      ____
                           _____
     _____
                                                           19930111 <--
                                           WO 1993-GB49
                            19930722
     WO 9314399
                      A1
PΙ
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                                                            19930111 <--
                                           EP 1993-901829
                       A1 19941026
     EP 620918
                            19970730
                       В1
     EP 620918
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
                                                            19930111 <--
                                           JP 1993-512258
                            19950323
                     Т2
     JP 07502817
                            20010625
                       В2
     JP 3178839
                                                            19930111 <--
                                           AT 1993-901829
                            19970815
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     AT 156269
                                                            19930111 <--
                                           ES 1993-901829
                       Т3
                            19971016
     ES 2105211
                                                            19940928 <--
                                           US 1994-256468
                       Α
                            19960102
     US 5480611
                                      <--
                            19920109
PRAI GB 1992-431
                       Α
                                      <--
                            19930111
     WO 1993-GB49
                       W
     A CO2 detector comprises an indicating member and a CO2 sensing medium and
AΒ
     is useful for medical uses, esp. trachea intubation. The indicating
     member comprises an intimate mixt. of a polymer vehicle (polyvinyl
     butyral, polyvinyl Me ether, etc.). The CO2 sensing medium comprises an
     anionic fluorimetric dye (1,3-dihydroxypyrene-6,8-disulfonate,
     fluorescein, etc.) and a lipophilic org. quaternary cation
      (benzyltrimethylammonium, trioctylmethylammonium, etc.). Thus, a film
     contg. 1-hydroxypyrene-3,6,8-trisulfonate, tetraoctylammonium, Et
      cellulose, and tris-Bu phosphate was coated on the surface of a gas
      impermeable tube. Exposure of the film to a high level of CO2 converted
      the deprotonated form of the dye into its protonated form, which can be
      monitored by measuring at 394nm.
      carbon dioxide detector fluorescent film; dye fluorescent carbon dioxide
 ST
      detector
      Polymers, uses
 IT
      RL: USES (Uses)
         (indicating membrane contg., in carbon dioxide detector)
      Vinvl acetal polymers
 IT
      RL: USES (Uses)
         (butyrals, indicating membrane contg., in carbon dioxide detector)
 ΙT
         (fluorescent, anionic, sensing medium contg., in carbon dioxide
         detector for medical use)
 IT
      Sensors
          (gas, for carbon dioxide, for medical use)
```

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IΤ
     124-38-9, Carbon dioxide, analysis
     RL: ANST (Analytical study)
         (detector for)
                605-45-8, Diisopropyl phthalate 56-81-5, Glycerine, uses
ΙT
     122-62-3
     70-55-3, p-Toluene sulphonamide 77-99-6, Trimethylolpropane 78-40-0,
     Triethyl phosphate
                           78-51-3
     RL: ANST (Analytical study)
        (in indicating membrane manuf. for carbon dioxide detector) 2-89-5, Poly(vinyl alcohol) 9003-09-2, Poly(vinyl methyl ether)
     9002-89-5, Poly(vinyl alcohol) 9003-09-2, Poly(vinyl methy 9003-53-6, Polystyrene 9004-32-4, Carboxymethyl cellulose
IT
     Ethylcellulose
                       9004-64-2, Hydroxypropyl cellulose
                                                             9004-67-5,
                       9011-14-7, Poly(methyl methacrylate)
     Methylcellulose
                                                                  25322-68-3,
     Polyethylene glycol
                             25322-69-4, Polypropylene glycol
                                                                  126-73-8
     Tributyl phosphate, uses
     RL: ANST (Analytical study)
         (indicating membrane contg., in carbon dioxide detector)
IT
     84-87-7, 1-Naphthol-4-sulfonic acid
                                              90-33-5
                                                         93-01-6,
                                    93-35-6, Umbelliferone
     2-Naphthol-6-sulfonic acid
                                                               567-18-0,
                                    583-17-5, 2-Hydroxycinnamic acid
                                                                         779-27-1,
     1-Naphthol-2-sulfonic acid
     7-Hydroxycoumarin-3-carboxylic acid 1214-24-0, 3,6-DiHydroxyxanthone
     2321-07-5, Fluorescein 3030-97-5, Salicylaldehyde semicarbazone 3722-51-8, 3-Hydroxyxanthone 6665-86-7, 7-Hydroxyflavone
     13057-72-2, 7-Hydroxyisoflavone 15463-09-9, 7-Hydroxylepidine
     20168-55-2, 3-Hydroxyacridone 27928-00-3 58851-99-3 85353-28-2
     85644-14-0
     RL: ANST (Analytical study)
         (sensing medium contg. fluorescent, in carbon dioxide detector)
                  10549-76-5, Tetrabutylammonium 14800-24-9,
IT
     Benzyltrimethylammonium 18198-39-5, Tetraphenylphosphonium
                                                                       19524-73-3,
                           20256-54-6, Tetrahexylammonium 22061-11-6
     Tetraoctylammonium
                   66997-36-2
     45306-06-7
     RL: ANST (Analytical study)
         (sensing medium contg., in carbon dioxide detector)
     13057-72-2, 7-Hydroxyisoflavone
TT
     RL: ANST (Analytical study)
         (sensing medium contg. fluorescent, in carbon dioxide detector)
RN
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
           0
     Ph
L50 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2003 ACS
     1993:185706 HCAPLUS
ΑN
DN
     118:185706
     Method using daidzin or daidzin analog for the inhibition of aldehyde
TΙ
     dehydrogenase I (ALDH-I), and use in the treatment of alcohol dependence
     or alcohol abuse
IN
     Vallee, Bert L.; Keung, Wing Ming
     Endowment for Research in Human Biology, Inc., USA
PΑ
SO
     PCT Int. Appl., 98 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
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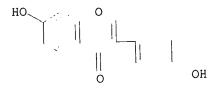
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ICM A61K031-35

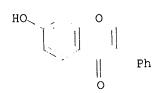
ICS C07D311-36; A61K031-70

4-7 (Toxicology) CC Section cross-reference(s): 7, 11, 27, 63 FAN.CNT 2 APPLICATION NO. DATE KIND DATE PATENT NO. \_\_\_\_\_ \_\_\_\_ 19920630 <--WO 1992-US5598 19930121 WO 9300896 A1 PΙ W: AU, BR, CA, FI, HU, JP, KR, NO, RO, RU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE 19910701 <--US 1991-723404 19930420 US 5204369 Α 19920630 <--AU 1992-23085 19930211 AU 9223085 Α1 19920630 <--EP 1992-915216 19940420 EP 592583 Α1 20010131 В1 EP 592583 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE AT 1992-915216 19920630 <--E 20010215 AT 198983 19920630 <--JP 1993-502339 20010528 B2 JP 3170281 19931230 <--NO 1993-4911 19940228 Α NO 9304911 US 1994-170272 19940524 <--19970429 Α US 5624910 US 1998-190360 19981112 <--В1 20010703 US 6255497 A2 19910701 <--PRAI US 1991-723404 19920630 <--WO 1992-US5598 Α 19940524 <--A1US 1994-170272 19970429 <--A3 US 1997-840360 MARPAT 118:185706 OS ALDH-I is inhibited by daidzin (I) or an analog thereof, optionally with ΆB factor(s) increasing the bioavailability of the I or I analog. Such inhibitory compds. or compns. are useful as pharmaceutical compns in methods for the treatment of alc. dependence (i.e. alcoholism) or alc. abuse, for alc. sensitization, for extinguishing an alc.-drinking response, for suppressing an urge for alc., for inducing alc. intolerance, for preventing alcoholism in an individual with or without a susceptibility or predisposition to alc. or alc. abuse, and for limiting alc. consumption in an individual, whether or not the individual is genetically predisposed. I was isolated from the crude drug Radix Puerariae (prepd. as the dried root of Pueraria lobata). Kinetic consts. for the inhibition by I of ALDH isoenzymes I and II were 40 and 20,000 nM, resp. Prepn. and inhibitory activity of ether derivs., e.g. daidzein 7-(.omega.-carboxydecyl) ether, is also presented. I, at doses of 5, 10, and 30 mg/day suppressed alc. intake by hamsters by 20, 50, and 80%, resp. I in a crude Radix Puerariae methanolic ext. was 5-10 times more potent than pure I. daidzin aldehyde dehydrogenase inhibitor; alcoholism treatment daidzin ST Drug bioavailability IT Solubility (daidzen compn. including factor increasing) Molecular structure-biological activity relationship IT (of aldehyde dehydrogenase I isoenzymes inhibition by daidzin and related compds.) Kinetics, enzymic IT(of aldehyde dehydrogenase I isoenzymes inhibition by daidzin and related compds., inhibition consts. for) . Drug dependence IT (alcoholism, treatment of, daidzin for, aldehyde dehydrogenase I inhibition in relation to) Kudzu IT (P. lobata, daidzin from Radix Puerariae of, aldehyde dehydrogenase I inhibition by, alcoholism treatment in relation to) IT Kudzu (P. lobata, roots, daidzin from, aldehyde dehydrogenase I inhibition by, alcoholism treatment in relation to) 552-66-9, Daidzin **486-66-8D**, analogs IT RL: BIOL (Biological study) (aldehyde dehydrogenase I inhibition with, alcoholism treatment in relation to)

525-82-6, Flavone 529-59-9, 486-62-4, Ononin 480-44-4, Acacetin 552-59-0, Prunetin 2555-30-8, 7-Hydroxy-4-phenylcoumarin IT Genistin 146699-00-5 146699-01-6 88407-29-8 36136-92-2 13057-72-2 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study) (aldehyde dehydrogenase inhibitory activity of) 9003-39-8, Polyvinylpyrrolidone 11024-24-1, Digitonin 25322-68-3, PEG ΙT RL: BIOL (Biological study) (daidzin soly. with) 7585-39-9, .beta.-Cyclodextrin ΙT RL: BIOL (Biological study) (daidzin soly. with PEG and) 64-17-5, Ethanol, biological studies IT RL: BIOL (Biological study) (intolerance to, induction of, daidzin for, aldehyde dehydrogenase I inhibition in relation to) 9028-86-8, Aldehyde dehydrogenase ΙT RL: BIOL (Biological study) (isoenzyme I, inhibition of, by daidzin or daidzin analog, alcoholism treatment in relation to) 146698-99-9P 146698-98-8P 146698-96-6P 146698-97-7P IT RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and aldehyde dehydrogenase I inhibitory activity of) 147158-76-7P 147158-74-5P 147158-75-6P IT RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of) 2834-05-1, .omega.-Bromoundecanoic acid 75-03-6, Ethyl iodide 4224-70-8, .omega.-Bromohexanoic acid 30515-28-7, .omega.-Bromoheptanoic ΙT acid RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with daidzin) **486-66-8D**, analogs IT RL: BIOL (Biological study) (aldehyde dehydrogenase I inhibition with, alcoholism treatment in relation to) 4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX 486-66-8 HCAPLUS RN CN NAME)



RL: BAC (Biological activity or effector, except adverse); BSU (Biological IΤ study, unclassified); BIOL (Biological study) (aldehyde dehydrogenase inhibitory activity of) 13057-72-2 HCAPLUS 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) RN CN



```
ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
AN
     1992:591584 HCAPLUS
DN
     117:191584
     An improved process for the preparation of substituted isoflavone
ΤI
     derivatives
     Kallay, Tamas; Lanyi, Gyorgy; Ledniczky, Laszlo; Fmrei, Lajos; Hoffmann,
IN
     Gyorgy; Sziladi, Maria; Somfai, Eva; Montay, Tibor
     Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.
PA
SO
     PCT Int. Appl., 22 pp.
     CODEN: PIXXD2
DΨ
     Patent
LA
     English
     ICM C07D311-36
IC
     A61K031-35
ICA
     26-4 (Biomolecules and Their Synthetic Analogs)
CC
FAN.CNT 1
     PATENT NO.
                       KIND
                             DATE
                                             APPLICATION NO.
                                                               DATE
                                             ______
                             19911017
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     WO 9115483
                       A1
         W: AU, CA, FI, JP, KR, NO, SU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE
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                             19911007
     AU 9054274
                        Α1
                             19911030
                                             AU 1990-54274
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                             19921210
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                                             EP 1990-906260
                                                               19900406 <--
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                        A1
                             19920408
                        В1
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     EP 478558
             AT, BE, CH, DE, DK, FR, GB, IT, LI, LU, NL, SE
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     JP 08009610
                        В4
                             19960131
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                             19940215
                                             NO 1991-4786
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     NO 9104786
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     US 5247102
                        Α
                             19930921
                                                               19911205 <--
                                             RU 1991-5010742
                                                               19911205 <--
     RU 2036918
                        C1
                             19950609
                                             LT 1993-779
                                                               19930713 <--
     LT 3463
                        В
                             19951025
PRAI EP 1990-906260
                             19900406
                                       <--
     WO 1990-HU23
                             19900406
                                       <---
     CASREACT 117:191584; MARPAT 117:191584
OS
GΙ
```

AB Isoflavones I (R = H, CHMe2; R1, R2 = H, OMe, OEt) were prepd. by cyclizing  $2,4-(HO)\,2C6H3COCH2C6H3R1R2$  with  $HC\,(OEt)\,3$  in the presence of base and, optionally alkylating I(R = H). Thus,  $2,4-(HO)\,2C6H3COCH2Ph$  was treated with  $HC\,(OEt)\,3$  and morpholine in HOCHMe2 to give 90.6% I (R-R2 = H) contg. 0.2-0.4% I (R = Et, R1, R2 = H).

ST hydroxyphenylacetophenone cyclization orthoformate; hydroxyisoflavone; isoflavone hydroxy

IT Cyclocondensation reaction

(of dihydroxyphenyl benzyl ketones with orthoformate, isoflavones by)

IT 122-51-0, Triethylorthoformate

RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclization of, with dihydroxyphenyl benzyl ketones)

```
138948-69-3
                 24126-98-5
ΙT
     3669-41-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (cyclization of, with orthoformate)
     138948-68-2P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and alkylation of)
                                                       35212-22-7P,
                                        24160-14-3P
     13057-72-2P, 7-Hydroxyisoflavone
IT
     7-Isopropoxyisoflavone 138948-70-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
     138948-68-2P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and alkylation of)
     138948-68-2 HCAPLUS
RN
     Carbonic acid, monopotassium salt, compd. with 7-hydroxy-3-phenyl-4H-1-
CN
     benzopyran-4-one potassium salt (1:1) (9CI) (CA INDEX NAME)
     CM
          1
          79130-53-3
     CRN
     CMF
         C15 H10 O3 . K
HO\
           0
                Ph
           0
          K
      CM
      CRN 298-14-6
      CMF C H2 O3 . K
    \circ
 HO-C-OH
   K
      13057-72-2P, 7-Hydroxyisoflavone
 ΙT
      RL: SPN (Synthetic preparation); PREP (Preparation)
          (prepn. of)
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4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

13057-72-2 HCAPLUS

RN

CN

L50 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1988:549354 HCAPLUS

DN

Preparation and formulation of 3-aryl-3,4-dihydro-2H-1-benzopyrans useful ΑN TIin treatment of vascular diseases

Albert, Alban Imre; Zilliken, Friedrich W. IN

Zyma S. A., Switz. PΑ

Eur. Pat. Appl., 23 pp. SO

CODEN: EPXXDW

Patent DT

LA

IC

ICM C07D311-58 ICS C07D493-04; C07D311-64; A61K031-35; A61K031-36

27-14 (Heterocyclic Compounds (One Hetero Atom)) CC

CC 27-14 (Heterocyc Section cross-re	ferenc	e(s): 1		
FAN.CNT 1 PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PT EP 267155	A A A A A2 A1 B2 A2 A	19880511 19880720 2, ES, FR, G 19880505 19880505 19900110 19880505 19880629 19890628 19880505 19910131 19880602 19880602	EP 1987-810620  B, GR, IT, LI, LU, NL NO 1987-4489 FI 1987-4804 DD 1987-308578 DK 1987-5756 ZA 1987-8245 HU 1987-4930 AU 1987-80655  JP 1987-277528 US 1987-116737	19871029 < 7, SE 79871028 < 19871102 < 19871103 < 19871103 < 19871104 < 19871104 < 19871104 <

Title compds. I [R = H, (un) substituted alkyl; one of R1 and R2 = H0, alkoxy, alkanoyloxy, alkyl and the other is H, or ORR1 = (un) substituted OCH2O; R2 = H, or ORR2 = (un)substituted OCH2O; B is (un)substituted by AΒ alkyl, phenylalkyl, alkanoyloxy, halo, amino, etc.] and their salts, useful for treatment of vascular diseases (no data) were prepd. 6,7-Dihydroxy-3-(3,4-dimethoxyphenyl)-4H-1-benzopyran-4-one in dioxane and

```
EtOH is hydrogenated for 8 days over Pd/C to give I [R, R2 = H, R1 = HO; B
     = 3,4-(Me20)2.
     aryldihydrobenzopyran prepn vascular disease treatment; benzopyran
ST
     aryldihydro prepn vascular disease
     Blood vessel, disease or disorder
IT
        (treatment of, aryldihydrobenzopyrans)
     Blood vessel, disease or disorder
        (Raynaud's phenomenon, treatment of, aryldihydrobenzopyrans for)
TT
     93-17-4, (3,4-Dimethoxyphenyl)acetonitrile
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (Friedel-Craft acylation of phenols by)
                                               459-22-3, (4-
     140-53-4, (4-Chlorophenyl)acetonitrile
IT
                                 501-00-8, (3-Fluorophenyl)acetonitrile
     Fluorophenyl)acetonitrile
                                             622-75-3, 1,4-
     555-21-5, (4-Nitrophenyl)acetonitrile
                            1529-41-5, (3-Chlorophenyl)acetonitrile
     Benzenediacetonitrile
     2338-76-3, (3-Trifluoromethylphenyl)acetonitrile 2947-60-6,
                                    2947-61-7, 4-Methylphenylacetonitrile
     (3-Methylphenyl) acetonitrile
     4395-87-3, (4-Isopropylphenyl)acetonitrile
                                                  5689-33-8
                                                               13288-86-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (Friedel-Craft acylation with phenols)
                                       533-73-3, 1,2,4-Trihydroxybenzene
                           136-77-6
     87-66-1, Pyrogallol
ΙT
     608-25-3, 2,6-Dihydroxytoluene
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (Friedel-Crafts acylation with acetonitriles)
                  116743-80-7
      93434-89-0
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclization of)
     3132-64-7, Epibromohydrin
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclocondensation of, with hydroxybenzopyranone deriv.)
      94105-89-2
 IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (esterification by, of acetic anhydride)
                   97148-44-2
      76397-87-0
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (esterification with, of acetic anhydride)
      3162-40-1
 ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification of, with Et bromobutyrate)
      533-68-6, Ethyl 2-bromobutyrate
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification of, with hydroxyphenylbenzopyranone deriv.)
      2051-90-3, Dichlorodiphenylmethane
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (etherification with, of dihydroxybenzopyran deriv.)
                                           37816-19-6 74693-73-5
                              36044-54-9
                  3162-32-1
      2746-87-4
 IT
                                            116703-48-1
                                                            116718-74-2
                   97284-26-9
                                 97770-37-1
      75187-63-2
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (hydrogenation of)
                                                                   116718-45-7P
                                                    116718-43-5P
                                     116718-42-4P
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      116718-40-2P
 IΤ
                                                                   116718-85-5P
                                                    116718-82-2P
                                     116718-76-4P
      116718-46-8P 116718-47-9P
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                                                    116718-99-1P
                                     116718-96-8P
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      116719-05-2P
                                                    116719-36-9P
                                     116719-31-4P
                      116719-27-8P
       116719-24-5P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
       (Reactant or reagent)
          (prepn. and cyclization of)
                                                                   116718-53-7P
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                                     116718-50-4P
       116718-48-0P
                      116718-49-1P
  ΙT
                                                                    116718-83-3P
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     (Reactant or reagent)
        (prepn. and hydrogenation of)
ΙT
     116719-30-3P
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     (Reactant or reagent)
        (prepn. and hydrolysis of)
     116718-52-6P
IT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and reactions of)
                    116718-56-0P
ΙT
     116718-54-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, as intermediate for benzopyrans for treatment of vascular
        diseases)
ΙT
     116719-37-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for treatment of muscular disease)
                    116718-58-2P
                                   116718-59-3P
                                                   116718-60-6P
                                                                  116718-61-7P
IT
     116718-44-6P
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                    116719-38-1P
     116719-35-8P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of, for treatment of vascular disease)
     98-09-9, Benzenesulfonyl chloride
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (sulfonylation by, of aminophenylbenzopyranone deriv.)
     75187-63-2
ΤT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (hydrogenation of)
     75187-63-2 HCAPLUS
RN
     4H-1-Benzopyran-4-one, 7,8-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX
CN
     NAME)
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L50 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2003 ACS

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AN 1988:523795 HCAPLUS
DN 109:123795
TI Cloning and sequencing of Bradyrhizobium japonicum nodD gene, recombinant
Bradyrhizobium or Rhizobium containing the gene, and flavones for inducing
expression of the gene
IN Appelbaum, Edward R.; Hennecke, Hauke; Lamb, Joseph W.; Gottfert, Michael
PA Lubrizol Genetics, Inc., USA
SO PCT Int. Appl., 90 pp.
CODEN: PIXXD2
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DT Patent LA English

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ICM C12N015-00
IC
     ICS C12N005-00; C07H015-12; A01H001-04
     3-4 (Biochemical Genetics)
CC
     Section cross-reference(s): 10, 11
FAN.CNT 2
                                        APPLICATION NO. DATE
                     KIND DATE
     PATENT NO.
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                           19871230
                                         WO 1987-US1421
                                                           19870617 <--
     WO 8707910
                     A1
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     AU 607928
PRAI US 1986-875297
                          19860617 <--
                           19870611 <--
     US 1987-61848
                           19870617
                                     <--
     WO 1987-US1421
     The nodD genes of Bradyrhizobium japonicum are isolated and sequenced.
AΒ
     These gene and recombinant DNA mols. contg. them are useful for
     engineering Rhizobium and Bradyrhizobium strains exhibiting enhanced
     competitiveness for nodulation, and for selective manipulation of
     nodulation host range of these strains. The nodD gene of B. japonicum
     USDA123 was isolated by genomic DNA screening using hybridization probes.
     Clone pEA5-1B contained two nodD open reading frames, designated nodD-1
     and nodD-2. A HindIII fragment of the B. japonicum USDA123 contg. nodD,
     the promoter region of nodD and nodA, and the amino terminal end of nodC
     was joined to the lacZ gene through nodC to produce plasmids pEA2-21 and
     pEA4-10. The fusion gene was inducible by soybean exudates and compds.
     such as 7-hydroxyisoflavone in B. japonicum contg. either of the plasmids.
     nodD gene Bradyrhizobium sequence cloning; hydroxyflavone nodD gene
ST
     Bradyrhizobium induction
IT
     Legume
     Soybean
        (exudates, induction of nodulation in recombinant Rhizobium or
        Bradyrhizobium contg. nodD gene with)
 ΙT
     Root nodule
         (formation induction of, in recombinant Rhizobium or Bradyrhizobium
        contq. nodD gene)
 ΙT
     Bradyrhizobium
     Rhizobium
         (nodulation gene promoter of, for nodD gene expression in recombinant
        Rhizobium or Bradyrhizobium)
     Molecular cloning
 TT
         (of nodD genes of Bradyrhizobium japonicum, in Escherichia coli)
      Bradyrhizobium japonicum
 TΤ
         (nodD gene of, cloning and sequencing of)
      Plasmid and Episome
 ΙT
         (pEA4-10, nodD-lacZ chimeric gene on, cloning and expression in
         Bradyrhizobium of)
      Plasmid and Episome
 IT
         (pRJ103, genes nodD1 and nodD2 of Bradyrhizobium japonicum on)
      Gene and Genetic element
 IT
      RL: BIOL (Biological study)
         (promoter, of nodulation gene of Rhizobium, for nodD gene expression in
         recombinant Rhizobium or Bradyrhizobium)
      Gene and Genetic element, microbial
 IT
      RL: BIOL (Biological study)
         (nodD, cloning and sequencing of, of Bradyrhizobium japonicum)
      Gene and Genetic element, microbial
 ΙT
      RL: BIOL (Biological study)
         (nodD1, cloning and sequencing of, of Bradyrhizobium japonicum)
      Gene and Genetic element, microbial
 IT
      RL: BIOL (Biological study)
         (nodD2, cloning and sequencing of, of Bradyrhizobium japonicum)
```

Operon IT

(nodABC, promoter of, of Bradyrhizobium japonicum, for nodD gene expression in recombinant Rhizobium or Bradyrhizobium)

116412-15-8, Protein (Bradyrhizobium japonicum clone pEA5-1B gene nodD2 ITreduced)

RL: PRP (Properties)

(amino acid sequence and cloning and expression of gene for)

116412-14-7, Protein (Bradyrhizobiúm japonicum clone pEA5-1B gene nodD1 IT reduced)

RL: PRP (Properties)

(amino acid sequence and expression of gene for)

116411-89-3, Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B 116411-90-6, Deoxyribonucleic acid (Bradyrhizobium japonicum ΙT gene nodD1) clone pEA5-1B gene nodD2)

RL: PRP (Properties)

(cloning and expression and nucleotide sequence of)

116411-91-7, Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B gene nodD1 plus 5'- and 3'-flanking region fragment) 116411-92-8, ΙT Deoxyribonucleic acid (Bradyrhizobium japonicum clone pEA5-1B gene nodD2 plus 5'- and 3'-flanking region fragment) RL: PRP (Properties); BIOL (Biological study)

(nucleotide sequence of)

446-72-0, Genistein 486-66-8, Daidzein ΙT

RL: PRP (Properties)

(nod gene induction with) 491-80-5 485-72-3, Formononetin Kaempferol 520-36-5, Apigenin 552-59-0, Prunetin 4044-00-2, TT 5,7-Dihydroxyisoflavone 13057-72-2, 7-Hydroxyisoflavone

(nodD gene induction with, in recombinant Bradyrhizobium or Rhizobium) RL: PRP (Properties)

446-72-0, Genistein 486-66-8, Daidzein IT

RL: PRP (Properties)

(nod gene induction with)

4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

IT

4044-00-2, 5,7-Dihydroxyisoflavone 13057-72-2,

7-Hydroxyisoflavone

RL: PRP (Properties)

(nodD gene induction with, in recombinant Bradyrhizobium or Rhizobium)

RN 4044-00-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)

RN 13057-72-2 HCAPLUS

CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)

L50 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2003 ACS

AN 1986:5774 HCAPLUS

DN 104:5774

TI Benzopyran-4-one derivatives

IN Yamazaki, Iwao; Sawa, Yoichi

PA Takeda Chemical Industries, Ltd., Japan

SO Eur. Pat. Appl., 18 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D311-36

ICS A61K031-35

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1, 63

FAN CNT 2

PAN.	CNT Z			
	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
ΡI	EP 146922	A2 1985070	3 EP 1984-115840	19841219 <
	EP 146922	A3 1986040	2	
	EP 146922	B1 1988090	7	
	R: BE, CH,	DE, FR, GB, IT	, LI, NL, SE	
	JP 60132976	A2 1985071		19831221 <
	HU 37138	0 1985112	B HU 1984-4748	19841220 <
	US 4644012	A 1987021	7 US 1984-684144	19841220 <
PRAI	JP 1983-242780	1983122	1 <	
	JP 1983-242779	1983122	1 <	
GI				

The title compds. I (R1 = H or OH; R2 = H or carboxyalkyl) prepd. by the reaction of I (R1 as above, R2 = H) with R3CHXCO2R4 (R3 = alkyl; R4 = H or AΒ alkyl; X = halo) in presence of an inert solvent and a deacidifying agent followed by hydrolysis of the ester obtained, are bone resorption inhibitors, and as such are useful in osteoporosis treatment. Thus, 7-hydroxy-3-phenyl-4H-1-benzopyran-4-one (I; R1 = R2 = H) was reacted with Et 2-bromopropionate in DMF in the presence of K2CO3 to give 7-[[1-(ethoxycarbonyl)ethyl]oxy]-3-phenyl-4H-1-benzopyran-4-one which was hydrolyzed to 7-[(1-carboxyethyl)oxy]-3-phenyl-4H-1-benzopyran-4-one (I; R1 = H, R2 = MeCHCO2H) (II). II demonstrated its effectiveness as bone resorption inhibitor in rat fetal long bone culture. A tablet formulation contained II 200, lactose 15, starch 45, Ca CM-cellulose 10, and Mg stearate 1 g, for 1000 uncoated tablets  $8.5\ \mathrm{mm}$  diam. phenylbenzopyranone prepn bone resorption inhibitor; carboxyalkylphenyl ST benzopyranone prepn pharmaceutical; osteoporosis treatment carboxyalkylphenylbenzopyranone prepn (resorption of, inhibitors of, [(carboxyethyl)oxy]phenylbenzopyranones) IΤ Osteoporosis IT(treatment of, [(carboxyethyl)oxy]phenylbenzopyranones for) 99007-90-6P 99007-87-1P IT RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and bone resorption-inhibiting activity of) 99007-85-9P 99007-86-0P 99007-84-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT IT (Reactant or reagent) (prepn. and hydrolysis of) 99007-88-2P 99007-89**-**3P ΙT RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, as bone resorption inhibitor) 13057-72-2 19725-36-1 89019-85-2 IT RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et bromopropionate) 486-66-8 IT RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ethylbromopropionate) 535-11-5 IT RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with hydroxyphenylbenzopyranones) 13057-72-2 19725-36-1 89019-85-2 ITRL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et bromopropionate) 13057-72-2 HCAPLUS 4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) RN CN

RN 19725-36-1 HCAPLUS CN 4H-1-Benzopyran-4-one, 7-hydroxy-3-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)

89019-85-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-(3-hydroxyphenyl)- (9CI) (CA INDEX CN NAME)

ΙT 486-66-8

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with ethylbromopropionate)

RN 486-66-8 HCAPLUS

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX CN

L50 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1985:583568 HCAPLUS

DN 103:183568

Use of 3-phenyl-4H-1-benzopyran-4-one derivatives for inhibiting and TIΙN

Tsuda, Masao; Sawa, Yoichi; Yamazaki, Iwao PΑ

Takeda Chemical Industries, Ltd. , Japan SO

Ger. Offen., 17 pp. CODEN: GWXXBX

DT Patent

LA

German IC ICM A61K031-35

CC 63-6 (Pharmaceuticals)

Section cross-reference(s): 1, 27

FAN.	0111 2	ererenc	e(s): 1, 27		
PI	PATENT NO.  DE 3446246	KIND	DATE	APPLICATION NO.	DATE
	JP 60132917 EP 146921 EP 146921	A1 A2 A2 A3	19850711 19850716 19850703 19860402	DE 1984-3446246 JP 1983-242779 EP 1984-115839	19841219 < 19831221 < 19841219 <
PRAI	R: BE, CH, US 4644012 JP 1983-242779	A	, GB, LI, NL, 19870217 19831221 <	SE US 1984-684144	19841220 <

JP 1983-242780 CASREACT 103:183568 19831221 <---

OS GΙ

I (R = CO2H, group convertible to CO2H; R1, R2 = H, alkyl; R3 = H, OH) inhibit bone resorption. Pharmaceuticals contg. I are effective in the AΒ prevention and treatment of osteoporosis caused by decreased estrogen secretion after menopause in women. I suppressed the bone resorption by .apprx.5%. Acute toxicity studies with mice and rats showed no death incidence and toxic symptoms. Thus, tablets were prepd., each contg. 200 mg I (R = CO2H, R1 = Me, R2 = R3 = H)(II) [99007-90-6]. II was prepd. by hydrolysis of the Et ester [99007-84-8] which was prepd. from  $\frac{1}{2}$ 7-hydroxy-3-phenyl-4H-1-benzopyran-4-one [13057-72-2] and Et 2-bromopropionate [535-11-5].

phenylbenzopyranone drug osteoporosis ST

Osteoporosis ΙT

(treatment of, phenylbenzopyranone derivs. for)

99007-86-0P 99007-84-8P 99007-85-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT IT (Reactant or reagent)

(prepn. and hydrolysis of)

99007-90-6P 99007-88-2P 99007-89-3P 99007-87-1P IT

RL: PREP (Preparation)

(prepn. of, for treatment of osteoporosis)

486-66-8 13057-72-2 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et bromopropionate)

535-11-5 IT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with hydroxyphenylbenzopyranones)

486-66-8 13057-72-2 TT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with Et bromopropionate)

4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)- (9CI) (CA INDEX RN CN NAME)

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) RN CN

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ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
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26-4 (Biomolecules and Their Synthetic Analogs) 514456000 NCL CC

Section cross-reference(s): 1

S	ection cross-re	ferenc	e(s): 1				
FAN.CN		KIND	DATE		APPLICATION NO.	DATE  1.9821115	<
U U PRAI U U	US 4501755 US 4495198 US 4668805 US 4668804 US 1981-259403 US 1982-422929 US 1981-259387 US 1981-330122 US 1982-441893	A A A A	19850226 19850122 19870526 19870526 19810501 19820924 19810501 19811214 19821115	< < < <	US 1982-441889 US 1982-441890 US 1986-885517 US 1986-885518	19821115 19821115 19860714 19860714	<
GI							

$$_{
m RR}$$
  $_{
m NCH}$   $_{
m 2CH}$   $_{
m (OH)}$   $_{
m CH}$   $_{
m 2O}$   $_{
m CH}$   $_{
m O}$   $_{
m I}$ 

- Isoflavones I (R = H, alkyl, cycloalkyl; R1 = H, Me; R2 = H, alkyl, CF3, cycloalkyl, furyl) were prepd. Thus 7-hydroxy-3-phenylchromone was treated with epichlorohydrin, followed by aminolysis with H2NCHMe2 to give AΒ I (R = CHMe2, R1 = R2 = H) which at 50 mg/kg orally gave 45% inhibition in
- phenylchromonyloxypropanolamine prepn antiinflammatory; propanolamine phenylchromonyloxy; isoflavone aminohydroxypropoxy ST
- Inflammation inhibitors and Antiarthritics IT

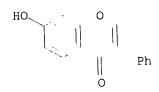
(isoflavonyloxypropanolamines)

ΙT

RL: RCT (Reactant); RACT (Reactant or reagent)

(aminolysis of epoxypropoxyisoflavone by) 97124-31-7P 84858-48-0P 84858-64-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT IT

```
(Reactant or reagent)
        (prepn. and aminolysis of)
                 84858-24-2P 84858-47-9P 84858-49-1P
                                                             84858-50-4P
    84858-22-0P
ΙT
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (prepn. and antiinflammatory activity of)
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
IT
     (Reactant or reagent)
        (prepn. and quaternization of)
                                                             97124-34-0P
                                               97124-33-9P
                   84858-45-7P 97124-32-8P
     84858-44-6P
IT
     97138-90-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. of)
                                                      97124-30-6
                                        84858-65-1
                          32131-70-7
     2859-88-3 13057-72-2
IΤ
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
     106-89-8, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
TΤ
        (reaction of, with hydroxyisoflavone)
     13057-72-2
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with epichlorohydrin)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
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L50 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2003 ACS
    1983:107161 HCAPLUS
AN
    98:107161
DN
    Antihypertensive agents
TI
    Wu, Edwin Shen Chou
IN
    Pennwalt Corp. , USA
PΑ
    Eur. Pat. Appl., 26 pp.
SO
    CODEN: EPXXDW
DΤ
    Patent
    English
LΑ
    C07D311-26; A61K031-35
TC
     27-14 (Heterocyclic Compounds (One Hetero Atom))
     Section cross-reference(s): 1, 63
FAN.CNT 4
                                      APPLICATION NO. DATE
     PATENT NO. KIND DATE
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                                       EP 1982-102950 19820406 <--
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     EP 64165
ΡI
                    B1 19870610
     EP 64165
        R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE
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                    Al 19850604
                                       AU 1982-80952 19820226 <--
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                    B2 19860626
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    US 4668805
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                                            US 1986-885518
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PRAI US 1981-259403
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     US 1981-330122
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                             19820406
     EP 1982-102950
                                       <--
                             19821115
     US 1982-441893
     CASREACT 98:107161
OS
GΙ
```

Antihypertensive chromones I (R = H, alkyl, cycloalkyl; R1 = H, alkyl, F3C, Ph, o-ClC6H4, p-ClC6H4; R2 = H, Ph; R3 = H, HO) were prepd. Thus, AΒ 7-hydroxy-2,3-diphenylchromone was treated with epichlorohydrin to give 7-(2,3-epoxypropoxy)-2,3-diphenylchromone, which was treated with Me2CHNH2 to give the chromone II. II had antihypertensive activity at 8 mg/kg in the spontaneously hypertensive rat.

chromone aminohydroxypropoxy; antihypertensive aminohydroxypropoxychromone

```
ST
     Antihypertensives
ΙT
        ((aminohydroxypropoxy)chromone)
                                                              84858-25-3P
                                                84858-23-1P
                                  84858-22-0P
                   76323-05-2P
                                                              84858-32-2P
     38186-01-5P
                                                84858-31-1P
IT
                                  84858-30-0P
                   84858-28-6P
                                                              84858-41-3P
     84858-27-5P
                                                84858-39-9P
                                  84858-38-8P
                   84858-36-6P
                                                               84858-50-4P
                                                84858-47-9P
     84858-34-4P
                                  84858-45-7P
                   84858-44-6P
     84858-43-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
                                  84858-57-1P
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
         (prepn. and antihypertensive activity of)
     37933-96-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
IT
         (prepn. and reaction of isopropylamine)
                                                               84858-60-6P
                                                 84858-48-0P
                                  84858-46-8P
                    84858-21-9P
      84858-19-5P
 IT
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction with isopropylamine)

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT ΙT (Reactant or reagent)

(prepn. and reaction with isopropylamines)

84858-42-4P RL: SPN (Synthetic preparation); PREP (Preparation) TT

```
(prepn. and reactions with isopropylamine)
                                               84858-29-7P 84858-33-3P
                  84858-20-8P
                                 84858-24-2P
IT
     84858-18-4P
                                               84858-53-7P 84858-54-8P
                                 84858-51-5P
     84858-35-5P
                   84858-37-7P
     84858-56-0P
                  84858-58-2P
                                 84858-59-3P
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        (prepn. of)
                           1003-03-8
IT
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     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with (epoxypropoxy)diphenylchromone)
     75-04-7, reactions 107-10-8, reactions 109-73-9, reactions
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IT
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        (reaction of, with (epoxypropoxy) flavone)
     75-31-0, reactions
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with (epoxypropyl)chromones)
                                                    18651-11-1
                             6665-86-7 13057-72-2
TT
     2859-88-3
                 6665-83-4
                               32131-70-7
                                           84858-62-8
     18651-15-5
                  22609-52-5
     84858-65-1
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
ΙT
     106-89-8, reactions
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with hydroxychromones)
     84858-26-4
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with isopropylamine)
TT
     13057-72-2
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with epichlorohydrin)
     13057-72-2 HCAPLUS
RN
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
CN
        Ph
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    ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2003 ACS
L50
     1981:550452 HCAPLUS
ΑN
DN
     95:150452
     Basic ethers and pharmaceutical preparations containing them
ΤI
     Hausberg, Hans Heinrich; Pruecher, Helmut; Uhl, Juergen; Seyfried,
TN
     Christoph; Minck, Klaus
     Merck Patent G.m.b.H. , Fed. Rep. Ger.
PΑ
     Ger. Offen., 41 pp.
SO
     CODEN: GWXXBX
DT
     Patent
     German
LA
     C07D311-36; C07D311-20; C07D311-22; C07D311-30
TC
     27-17 (Heterocyclic Compounds (One Hetero Atom))
CC
     Section cross-reference(s): 26
FAN.CNT 1
                                            APPLICATION NO.
                                                             DATE
                      KIND DATE
     PATENT NO.
                                                             19791213 <--
                                            DE 1979-2950135
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                                            EP 1980-107005
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     EP 31885
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R: AT, BE, CH, DE, FR, GB, IT, NL, SE

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AT 1980-107005
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    AU 536811
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                              19791213
PRAI DE 1979-2950135
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     EP 1980-107005
                                        <--
                              19801215
     US 1980-216454
                              19830121
                                        <--
     US 1983-459928
                              19850211
     US 1985-700226
GI
```

Basic ethers I (R = MeNR2CH2CH2CHR1, Q, Q1, Q2; R1 = cyclopropyl, R5; R2 = H, C1-4 alkyl, C2-4 alkenyl, C4-8 cycloalkylalkyl, PhCH2; R3 = H, R5; R4 = AB H, C1-4 alkyl; R5 = Ph, optionally substituted with F, C1, C1-4 alkoxy or alkylthio, OCH2O, CF3; X = OCHR6CHR7CH2, OCHR6CHR7CO, OCR6:CR7CO, CH2CHR6CHR7CO; R6, R7 = H, C1-4 alkyl, C3-6 cycloalkyl, R5), useful as antidepressants (no data), were prepd. A soln. of 7-hydroxyisoflavone in ethanolic KOH was evapd. and the residue in DMF treated with PhCHClCH2CH2NMe2 in DMF at 150.degree. to give (aminopropoxy)isoflavone

amino ether antidepressant prepn; isoflavone aminopropoxy antidepressant ST prepn; aminopropoxyisoflavone antidepressant prepn

Antidepressants IT

(amino ethers)

13057-72-2 IT

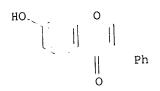
RL: PROC (Process)

(conversion of, to potassium salt)

79130-67-9P IT

```
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. and debenzylation of)
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
ΙT
        (prepn. and reaction of, with aminochloropropane deriv.)
     (Reactant or reagent)
                                                              79130-57-7P
                                 79130-55-5P
                                                              79130-62-4P
                   79130-54-4P
     79130-52-2P
                                                79130-61-3P
                                  79130-60-2P
TΤ
                   79130-59-9P
                                                              79130-68-0P
                                                79130-66-8P
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     79130-69-1P
                                  79130-76-0P
                   79130-75-9P
                                                              79130-83-9P
                                                79130-82-8P
     79130-74-8P
                                  79130-81-7P
                   79130-80-6P
                                                              79130-88-4P
                                                79130-87-3P
     79130-79-3P
                                  79130-86-2P
                                                               79130-94-2P
                    79130-85-1P
     79130-84-0P
                                                79130-93-1P
                                  79130-91-9P
                                                               79130-99-7P
                    79130-90-8P
                                                79130-98-6P
     79130-89-5P
                                  79130-97-5P
                    79130-96-4P
     79130-95-3P
                    79137-17-0P
     RL: SPN (Synthetic preparation); PREP (Preparation)
                                                           79131-04-7
         (prepn. of)
                                              79131-03-6
                                79131-02-5
                                           79131-08-1 79131-09-2
                   79131-01-4
      79131-00-3
                              79131-07-0
 IT
      79131-05-8 79131-06-9
                                                           79131-14-9
                                              79131-13-8
                                79131-12-7
                   79131-11-6
      79131-10-5
                                79137-18-1
                   79131-16-1
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction of, with aminohalo compd.)
                    79131-18-3
      RL: RCT (Reactant); RACT (Reactant or reagent)
 IT
          (reaction of, with aminopropyl chloride deriv.)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  TT
          (reaction of, with hydroflavone sodium salt)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  IT
          (reaction of, with hydroxychroman sodium salt)
                             5911-08-0
       106-95-6, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
  IT
          (N-alkylation by, of (aminopropoxy)isoflavone deriv.)
       RL: RCT (Reactant); RACT (Reactant or reagent)
  IT
           (N-methylation of)
        RL: RCT (Reactant); RACT (Reactant or reagent)
   TT
           (O-alkylation by, of hydroxyisoflavone)
        13057-72-2
   IT
        RL: PROC (Process)
           (conversion of, to potassium salt)
        4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
        13057-72-2 HCAPLUS
   RN
   CN
   HO_
              0
                    Ph
               0
         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    IT
             (prepn. and reaction of, with aminochloropropane deriv.)
         (Reactant or reagent)
          79130-53-3 HCAPLUS
    RN
```

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, potassium salt (9CI) (CA CN INDEX NAME)



K

79131-06-9 ΙT

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with aminohalo compd.)

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl-, sodium salt (9CI) (CA INDEX 79131-06-9 HCAPLUS RNCN NAME)



Na

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L50 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2003 ACS
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1980:6415 HCAPLUS AN

92:6415 DN

Animal feed containing anabolic isoflavones

Feuer, Laszlo; Nogradi, Mihaly; Gettsegen, Agnes; Vermes, Borbala; Strelisky, Janos; Wolfner, Andras; Farkas, Lorant; Antus, Sandor; Toth, ΤI IN

Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., USA

U.S., 8 pp. Cont.-in-part of U.S. 3,833,730. PΑ SO CODEN: USXXAM

DTPatent

English LA

A61K031-35 IC

NCL 424283000 27-15 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 18

CC	Section cross-re	ferenc	e(s): 18			
FAN.	CNT 3 PATENT NO.	KIND	DATE		APPLICATION NO.	DATE
PI PRAI	US 4166862 US 3833730 US 3907830 US 3864362 US 3949085 US 1971-146773 HU 1970-C1996	A A A A A	19790904 19740903 19750923 19750204 19760406 19710525 19700527	<	US 1974-470444 US 1971-146773 US 1973-371560 US 1973-374056 US 1974-497644	19740516 < 19710525 < 19730619 < 19730627 < 19740815 <

```
US 1973-371560
                                19730619 <--
         7-Hydroxy-2-methylisoflavone and 7-hydroxyisoflavone ethers, which were
    AB
         prepd. from 2,4-dihydroxyphenyl benzyl ketone 4-ethers, showed their
         effectiveness as animal feed wt.-gaining additives. A mixt. of
        2,4-HO(Me2CHO)C6H3COCH2Ph, HC(OEt)3, morpholine, and DMF was refluxed 8 h,
        with removal of the EtOH formed, to give 7-isopropoxyisoflavone.
        alkoxyisoflavone prepn animal growth; benzoyloxyisoflavone prepn animal
        growth; isoflavone alkoxy prepn animal growth
   IT
            (additives for, hydroxyisoflavone ethers as)
        Animal growth substances
        RL: RCT (Reactant); RACT (Reactant or reagent)
           (hydroxyisoflavone ethers)
   ΙT
        557-21-1
        RL: RCT (Reactant); RACT (Reactant or reagent)
           (cyclocondensation reaction of hydrogen cyanide from, with
           o-hydroxyphenyl benzyl ketones)
   ΙT
        72111-19-4
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (cyclocondensation reaction of, with acetic anhydride, isoflavone
           deriv. from)
       18439-96-8
  IT
       RL: RCT (Reactant); RACT (Reactant or reagent)
           (cyclocondensation reaction of, with ethoxalyl chloride)
  IT
       50561-04-1
       RL: RCT (Reactant); RACT (Reactant or reagent)
                                  50775-76-3
          (cyclocondensation reaction of, with orthoformate ester)
  TΤ
       68-12-2, reactions
       RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketone
          deriv.)
       109-94-4
                  122-51-0
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones)
 IΤ
      4755-77-5
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones,
         decarboxylation in)
 IT
      108-24-7
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (cyclocondensation reaction of, with o-hydroxyphenyl benzyl ketones,
         isoflavones from)
 ΙT
      54585-89-6P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (prepn. and dehydration of)
TΤ
      35212-47-6P
                    35212-50-1P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
         (prepn. and sapon. of)
ΙT
     35212-22-7P
                    35212-28-3P
                                  35212-32-9P
                                                35212-33-0P
     35212-42-1P
                                                              35212-35-2P
                   35212-52-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (prepn. and use of, in animal feed)
ΙT
     844-95-1P
                23915-78-8P
                               35212-24-9P
                                              35212-25-0P
     35212-29-4P
                                                            35212-26-1P
                   35212-30-7P
                                 35212-31-8P
                                                35212-34-1P
     35212-37-4P
                                                              35212-36-3P
                   35212-38-5P
                                 35212-39-6P
                                                35212-40-9P
     35212-43-2P
                                                              35212-41-0P
                   35212-44-3P
                                 35212-45-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
                                                35212-46-5P
                                                              35294-02-1P
        (prepn. of)
IT
     13057-73-3
                  54528-15-3
                               54528-35-7
    RL: RCT (Reactant); RACT (Reactant or reagent)
                                            54528-37-9
                                                          54528-40-4
        (use of, in animal feed)
```

```
2859-88-3 13057-72-2
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of)
               3145-86-6
     111-25-1
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavone by)
     100-44-7, reactions
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavone deriv. by)
     78-76-2
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of hydroxyisoflavones by)
     13057-72-2
ΙT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (O-alkylation of)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
           0
                Ph
           0
 L50 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2003 ACS
      1977:405809 HCAPLUS
 AN
      4-Oxo-4H-benzopyran derivatives useful in fodder compositions
 DN
 TΙ
      Bass, Robert John
 IN
      Pfizer Corp., Panama
 PΑ
      Ger. Offen., 20 pp.
 SO
      CODEN: GWXXBX
 DT
      Patent
      German
 LA
      C07D311-36
 IC
      27-14 (Heterocyclic Compounds (One Hetero Atom))
 CC
      Section cross-reference(s): 18
 FAN.CNT 1
                                           APPLICATION NO. DATE
                       KIND DATE
      PATENT NO.
                                           _____
                             _____
      _____
                                          DE 1976-2640617 19760909 <--
                             19770317
      DE 2640617
                       A1
                                                            19750912 <--
  PΤ
                                           GB 1975-37553
                       A
                             19771214
      GB 1495189
                                                            19760910 <--
                      A1
                                           BE 1976-170560
                           19770310
      BE 846109
                                                            19760910 <---
                                           DK 1976-4119
                            19770313
                       Α
      DK 7604119
                       A 19770315
A 19770315
                                                            19760910 <--
                                           NL 1976-10059
      NL 7610059
                                                            19760910 <--
                                           JP 1976-108684
                       A2 19770511
       JP 52057182
                                                            19760910 <--
                                           FR 1976-27339
                       A1 19770527
       FR 2329269
                                                            19770510 <--
                                           US 1977-795652
                            19780926
                       A
       US 4117149
                             19750912 <--
  PRAI GB 1975-37553
                             19760813 <--
```

US 1976-714086

GΙ

```
Ι
     Benzopyranones (I; R = H, OH, Me, MeO; R1 = H, Cl, OH; R2 = H, OH, Me,
     MeO; R3 = e.g. Ph, 4-MeC6H4, 4-PhC6H4, PhSO2, PhCH2, 4-MeOC6H4O,
AB
     cyclopentyl, 2-naphthyl), useful as animal growth substances, are prepd.
     by reaction of 2'-hydroxyacetophenones with DMF or MeCONMe2 in presence of
     MeSO2Cl and BF3.Et2O. Thus, reaction of 2,4,6-(HO)3C6H2COCH2C6H4Me-4 with DMF 2 h at 100.degree. gives 85% I (R = R2 = OH, R1 = H, R3 = 4-MeC6H4).
     benzopyranone animal growth prepn
ST
     Animal growth substances
ΤТ
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (benzopyranone derivs.)
     485-72-3P 491-80-5P 4044-00-2P 13057-72-2P
                                                                 59108-72-4P
IT
                                                  59108-71-3P
                                  15584-09-5P
                    15584-08-4P
     15584-07-3P
                                                                 62845-08-3P
                                                  62845-07-2P
                                   59297-07-3P
                    59108-74-6P
     59108-73-5P
                                                                 62845-13-0P
                                                  62845-12-9P
                                   62845-11-8P
                    62845-10-7P
     62845-09-4P
                                                                 62845-18-5P
                                                  62845-17-4P
                                   62845-16-3P
                    62845-15-2P
      62845-14-1P
                                             62845-22-1P
      62845-19-6P 62845-20-9P 62845-21-0P
                                   62881-65-6P
                    62881-64-5P
      62845-23-2P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
      124-63-0
ΙT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of hydroxyacetophenone derivs. with dimethylformamide or
         dimethylacetamide in presence of borontrifluoride etherate and)
      109-63-7
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of hydroxyacetophenone derivs. with dimethylformamide or
         dimethylacetamide in presence of methanesulfonyl chloride and)
      127-19-5
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction with (fluorophenyl)trihydroxyacetophenone)
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction with dimethylacetamide)
      59108-68-8
 IT
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction with dimethylformamide)
      68-12-2, reactions
 TΤ
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (reaction with trihydroxytolylacetophenone)
       4044-00-2P 13057-72-2P 62845-20-9P
 IT
       62845-21-0P
       RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of)
4044-00-2 HCAPLUS
       4H-1-Benzopyran-4-one, 5,7-dihydroxy-3-phenyl- (9CI) (CA INDEX NAME)
  RN
  CN
```

13057-72-2 HCAPLUS RN

4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME) CN

62845-20-9 HCAPLUS RN

4H-1-Benzopyran-4-one, 5-hydroxy-3-(4-hydroxyphenyl)-7-methyl- (9CI) (CA CN INDEX NAME)

62845-21-0 HCAPLUS

RN4H-1-Benzopyran-4-one, 7-hydroxy-3-(4-hydroxyphenyl)-5-methyl- (9CI) (CA CNINDEX NAME)

L50 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2003 ACS

1975:16704 HCAPLUS ΑN

82:16704 DN

Catabolic 7-alkoxyisoflavones as feed additives

TIFeuer, Laszlo; Nogradi, Mihaly; Gottsegen, Agnes; Vermes, Borbala; Streliszky, Janos; Wolfner, Andras; Farkas, Lorant; Antus, Sandor; Kovacs, ΙN

Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt. PΑ

Ger. Offen., 23 pp. Division of Ger. Offen. 2,125,245 (CA 76: 72407e). SO CODEN: GWXXBX

DTPatent

German LA

A61K; A23K IC

27-15 (Heterocyclic Compounds (One Hetero Atom)) CC Section cross-reference(s): 5

FAN.CN	T 3 ATENT NO.	KIND	DATE	<u> P</u>	APP	LICATION NO.	DATE	
_				_		1071 2166459	19710521	<b></b>
	E 2166458	A1	19741003			1971-2166458 1970-CI996	19710521	
	U 162377	P	19730228 19751015			1971-36929	19710520	
	L 36929 E 2166085	Al Al	19731013			1971-2166085	19710521	
	E 2166085	B2	19790816	-		17,1 010000		
	E 2166085	C3	19800424					
	T 311342	В	19731112	F	TF	1971-444	19710524	
	т 311778 .	В	19731210			1971-10281	19710524	
	Т 318613	В	19741111			1972-6909	19710524	
	S 391486	A1	19750301			1971-391486	19710524	
	L 7107128	A	19711130	1	NL	1971-7128	19710525	<
	L 170539	В	19820616				•	
N	L 170539	С	19821116	_		1071 6745	10710505	
	E 389001	В	19761025			1971-6745	19710525 19710526	
	U 402176	D	19731012			1971-1667729	19710526	
	B 1360461	A	19740717			1971-17293 1974-1583	19710526	
	B 1360462	A	19740717			1974-1363	19710526	
	CH 565786	A	19750829			1971-7704	19710526	
	CH 567499	A	19751015 19760325			1971-1717079	19710526	
	SU 508205	D P	19760430			1971-160121	19710526	
	PL 84997 NO 134239	В	19760531			1971-1986	19710526	
	OK 137362	В	19780227	j	DK	1971-2543	19710526	
	PL 98591	P	19780531		PL	1971-148411	19710526	<
	PL 99030	P	19780630			1971-175267	19710526	
	R 2100692	A5	19720324			1971-19257	19710527	
	CS 157871	В	19741015			1971-3888	19710527	
	CS 165839	В	19751222			1971-6392	19710527	
	CA 998057	A1	19761005			1971-114041	19710527	
H	RO 62749	P	19770915			1971-70509	19710527 19710527	
Ċ	JP 54013391	B4	19790530			1971-35940		
	FI 57406	В	19800430		F.T	1971-1463	19710527	<b>\</b>
	FI 57406	C	19800811		TO CO	1971-398289	19711223	<
	ES 398289	A1	19750416			1973-371560	19730619	
	JS 3907830	A	19750923 19750204			1973-374056	19730627	
	JS 3864362	A A1	19760616			1974-425900	19740502	
	ES 425900 SE 7407325	A	19740604			1974-7325	19740604	
	SE 412586	Ĉ	19800626					
	US 3949085	Ā	19760406			1974-497644	19740815	
	CA 986355	A2	19760330		CA	1975-217729	19750110	
	DK 7601789	Α	19760421		DK	1976-1789	19760423	<
	DK 143651	В	19810921					
	DK 143651	С	19820222			1000 115001	1077000	7 /
	JP 53053657	A2	19780516		JP	1977-115994	1977092	/ <
	JP 59003998	B4	19840127			1070 1700	1979052	2 /
	FI 7901702	A	19790528		ΕŢ	1979-1702	19/9032	,
	FI 64045	B	19830630					
	FI 64045	C	19831010 19840410		ΤD	1982-216782	1982121	) <
	JP 59062581	A2	19840410		Οſ	1702 210102	1002122	
	JP 59025791	B4	19700527	<				
	HU 1970-CI996 US 1971-146773			<				
	DK 1971-2543			<				
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	US 1973-371560		19730619	<				
O.T.	Tree diamon/al	see p	rinted CA I	ssue.			. 10.1 17	Mo
AB	Thout 10 isofla	MODES	II. $Rn = H$ .	(OMe)	) 2-	-3,4, or $NOZ-4$	F : KL = H,	Me, OI H2CH2
	CO2H; $R2 = e.g.$	C1-11	. alkyl, PhC	HZ, 4	-C]	CON4CHZ, ECUZ	.CCHZ, HOC	11201121

ST

ΙT

IT

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TΤ

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EtOCH2CH2, or 3-pyridylpropyl] were prepd. and (or) used as catabolic feed
  additives. Thus, 2,4-HO(Me2-CHO)C6H3COCH2Ph and HC(OEt)3 were refluxed in
  DMF contg. morpholine to give I (Rn = R1 = H, R2 = Me2CH).
   2,4-HO-(BuO)C6H3COCH2Ph was refluxed in Ac2O contg. AcONa to give I (Rn =
   H, R1 = Me, R2 = Bu). I (Rn = R1 = R2 = H) and hexyl bromide were
   refluxed in Me2CO contg. K2CO3 and KI to give I (Rn = R1 = H, R2 = hexyl).
   2,4-HO(MeO)C6H3CO-CH2Ph reacted with ClCOCO2Et in pyridine to give Et
   2,3-dihydro-2-hydroxy-7-methoxyisoflavone-2-carboxylate, which on heating
   with concd. HCl gave I (Rn = H, R1 = CO2Et, R2 = Me) (II). II was
   hydrolyzed in aq. NaOH and Me2CO to give I (Rn = H, R1 = CO2H, R2 = Me).
   feed additive catabolic isoflavone; alkoxyisoflavone feed additive;
   pyridylpropoxyisoflavone feed additive
   Feed
      (additives, catabolic alkoxyisoflavones as)
                                                        54528-35-7
                                           54528-15-3
                             54510-03-1
                50776-06-2
   13057-73-3
                                                        54585-86-3
                                           54528-40-4
                             54528-38-0
                54528-37-9
   54528-36-8
   RL: RCT (Reactant); RACT (Reactant or reagent)
      (catabolic feed additive)
                                                4755-77-5
                                     557-21-1
                         122-51-0
              109-94-4
   108-24-7
   RL: RCT (Reactant); RACT (Reactant or reagent)
       (cyclization of benzyl phenyl ketones and)
                             50775-76-3
                50775-75-2
   50561-04-1
   RL: RCT (Reactant); RACT (Reactant or reagent)
       (cyclization with formic acid derivs.)
                                                            35212-42-1P
                                              35212-35-2P
                                35212-33-0P
                  35212-32-9P
   35212-22-7P
   35212-52-3P
                  54851-23-9P
   RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. and catabolic activity of)
   RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (prepn. and dehydration of)
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
    (Reactant or reagent)
       (prepn. and hydrolysis of)
                                                             35212-29-4P
                                               35212-28-3P
                                35212-26-1P
                  35212-25-0P
    35212-24-9P
                                                             35212-37-4P
                                               35212-36-3P
                                 35212-34-1P
                  35212-31-8P
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                                                             35212-43-2P
                                               35212-41-0P
                                35212-40-9P
                  35212-39-6P
    35212-38-5P
                                               54528-34-6P
                                35294-02-1P
                  35212-51-2P
    35212-44-3P
    RL: SPN (Synthetic preparation); PREP (Preparation)
       (prepn. of)
    2859-88-3 13057-72-2
                           54528-39-1
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with alkyl halides)
    10025-87-3
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with dimethylformamide)
    18439-96-8
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with ethyl (chlorocarbonyl) formate)
                                     3145-86-6
                         111-25-1
               100-44-7
     78-76-2
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with hydroxyisoflavones)
     68-12-2, reactions
TT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (with phosphoryl chloride)
     13057-72-2
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with alkyl halides)
     13057-72-2 HCAPLUS
     4H-1-Benzopyran-4-one, 7-hydroxy-3-phenyl- (9CI) (CA INDEX NAME)
RN
CN
```

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Waehaelae, Kristina; Hase, Tapio; Adlercreutz, Herman
ΑU
     Dep. Chemistry, Univ. Helsinki, Helsinki, FIN-00014, Finland
CS
     Proceedings of the Society for Experimental Biology and Medicine (1995),
SO
     208(1), 27-32
     CODEN: PSEBAA; ISSN: 0037-9727
PB
     Blackwell
DT
     Journal
LA
     English
     26-4 (Biomolecules and Their Synthetic Analogs)
CC
     The synthesis of the important diphenolic isoflavone type of
AΒ
     phytoestrogens starting from the corresponding unprotected phenols and
     arylacetic acids is discussed. The aryl rings may carry addnl. alkyl,
     methoxy, and/or halogeno groups. Intermediate polyhydroxydeoxybenzoins
     can also be isolated in good yield. Isotopically labeled isoflavone
     phytoestrogens were prepd. by H/D exchange in the complete mol. By this
     method the deuterated products are available in an isotopic purity of
     .gtoreq.90%.
     isoflavone; arylacetate phenol acylation; deuteration daidzein genistein
ST
     Flavonoids
ΙT
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (iso-, oxo, prepn. and labeling of isoflavones from phenols and
        arylacetic acids)
     104-01-8, 4-Methoxyphenylacetic acid
IT
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                     136466-47-2P
IT
     104411-13-4P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. and labeling of isoflavones from phenols and arylacetic acids)
                                    93-25-4, 2-Methoxyphenylacetic acid
     87-66-1, 1,2,3-Benzenetriol
IT
                                          103-82-2, Phenylacetic acid, reactions
     95-88-5, 4-Chloro-1,3-benzenediol
                                            108-46-3, 1,3-Benzenediol, reactions
     106-44-5, 4-Methylphenol, reactions
                                                                   120-80-9,
     108-73-6, 1,3,5-Benzenetriol
                                     108-95-2, Phenol, reactions
                                   156-38-7, 4-Hydroxyphenylacetic acid
     1,2-Benzenediol, reactions
     306-08-1, 4-Hydroxy-3-methoxyphenylacetic acid
                                                      504-15-4,
                                                                608-25-3,
                                 533-73-3, 1,3,4-Benzenetriol
     5-Methyl-1, 3-benzenediol
                                 614-75-5, 2-Hydroxyphenylacetic acid
     2-Methyl-1,3-benzenediol
                                             1798-09-0, 3-Methoxyphenylacetic
      621-37-4, 3-Hydroxyphenylacetic acid
     acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (prepn. of isoflavones from phenols and arylacetic acids)
                                                         15485-65-1P
                                           3669-41-8P
 16-2 457-49-0F - -217(531-8P
                               2491-32-9P
                                                              89019-84-1P
                                                89019-83-0P
                                  77316-95-1P
      17720-60-4P
                    40456-49-3P
                                                  139256-04-5P
                                                                 150295-88-8P
                                   139256-03-4P
                    139256-02-3P
      RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
      (Reactant or reagent)
         (prepn. of isoflavones from phenols and arylacetic acids)
                             485-72-3P, 7-Hydroxy-4'-methoxyisoflavone
      446-72-0P, Genistein
 IT
                            491-80-5P, 5,7-Dihydroxy-4'-methoxyisoflavone
      486-66-8P, Daidzein
                                                                    13057-72-2P,
                             4044-00-2P, 5,7-Dihydroxyisoflavone
      574-12-9P, Isoflavone
                            19725-36-1P
                                          21913-98-4P
                                                        62845-21-0P
      7-Hydroxyisoflavone
                                                                   89019-85-2P
      63909-40-0P, 7-Hydroxy-2'-methoxyisoflavone
                                                    75187-63-2P
                                   139256-06-7P 139256-07-8P
                     139256-05-6P
      118024-87-6P
      139256-08-9P
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of isoflavones from phenols and arylacetic acids)
      139256-07-8P
 IT
      RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of isoflavones from phenols and arylacetic acids)
      139256-07-8 HCAPLUS
 RN
      4H-1-Benzopyran-4-one, 6-chloro-7-hydroxy-3-(4-hydroxyphenyl)- (9CI)
 CN
      INDEX NAME)
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HO. O OH
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IT

87-66-1, 1,2,3-Benzenetriol

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ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS
L15
     1992:105915 HCAPLUS
ΑN
     116:105915
DN
ΤI
     Expedient synthesis of polyhydroxyisoflavones
     Wahala, Kristiina; Hase, Tapio A.
ΑU
     Dep. Chem., Univ. Helsinki, Helsinki, SF-00100, Finland
CS
SO
     Journal of the Chemical Society, Perkin Transactions 1:
     Bio-Organic Chemistry (1972-1999) (1991), (12), 3005-8
     CODEN: JCPRB4; ISSN: 0300-922X
DT
     Journal
LA
     English
CC
     26-4 (Biomolecules and Their Synthetic Analogs)
OS
     CASREACT 116:105915
     Polyhydroxyisoflavones (19 compds.) were prepd. by reaction of unprotected
AΒ
     phenols with arylacetic acid in the presence of BF3. Et2O followed by
     treatment with MeSO2C1. In many cases the intermediate deoxybenzoins were
     also isolated.
ST
     isoflavone polyhydroxy; deoxybenzoin polyhydroxy; phenol arylacetate
     condensation
IT
     Flavonoids
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (iso-, hydroxy oxo, polyhydroxy-, prepn. of, from unprotected phenols
        and arylacetic acids)
IT
     1835-11-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (oxidn. of)
IT
     487-49-0P
                 2491-31-8P
                               2491-32-9P
                                            3669-41-8P
                                                         15485-65-1P
                                                77316-95-1P
                    40456-49-3P
                                  52122-86-8P
                                                               89019-83-0P
     17720-60-4P
                   92549-46-7P
                                  139256-01-2P
                                                 139256-02-3P
                                                                 139256-03-4P
     89019-84-1P
     139256-04-5P
     RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and intramol. cyclocondensation of)
IT
     306-08-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
         (prepn. and reaction of, with phenols)
IT
     67736-18-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of)
                                          491-80-5P
                              486-66-8P
                                                      574-12-9P, Isoflavone
IT
     446-72-0P
                  485-72-3P
                                                              32684-57-4P
                   13057-72-2P
                                 19725-36-1P
                                               21913-98-4P
     4044-00-2P
                    63909-40-0P
                                  75187-63-2P
                                                89019-85-2P
                                                               118024-87-6P
     62845-21-0P
                     139256-06-7P 139256-07-8P
                                                 139256-08-9P
     139256-05-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
         (prepn. of, from phenol and phenylacetic acid)
     93-25-4, 2-Methoxyphenylacetic acid
                                            103-82-2, Phenylacetic acid,
IT
                  104-01-8, 4-Methoxyphenylacetic acid
                                   614-75-5, 2-Hydroxyphenylacetic acid
     4-Hydroxyphenylacetic acid
                                             1798-09-0, 3-Methoxyphenylacetic
     621-37-4, 3-Hydroxyphenylacetic acid
     acid
     RL: RCT (Reactant); RACT (Reactant or reagent)
         (reaction of, with phenols)
```

95-88-5, 4-Chloro-1, 3-benzenediol